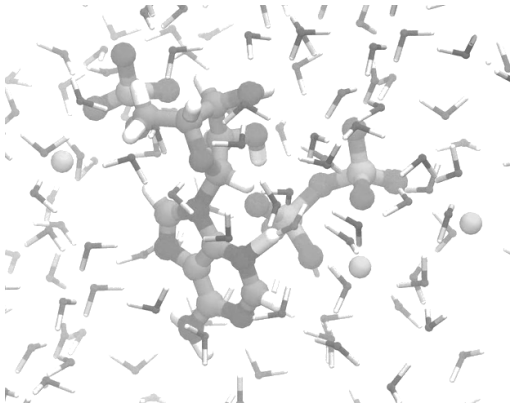
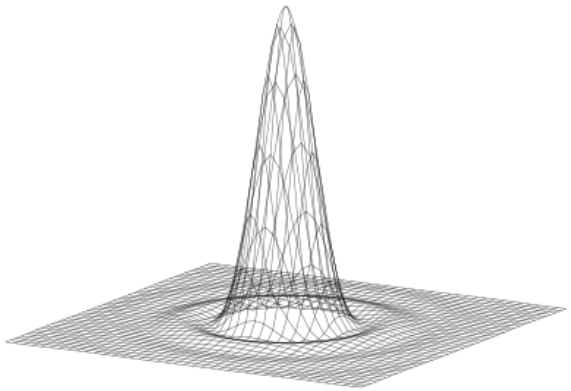
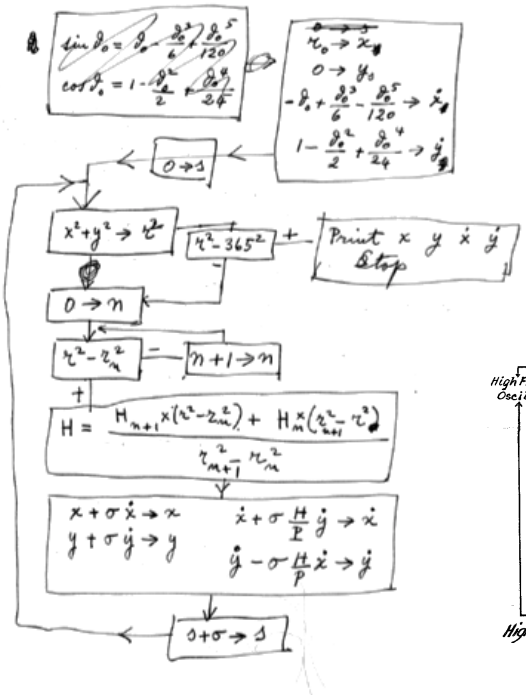
The XXIXth IUPAP Conference on Computational Physics

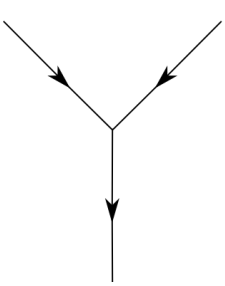
CCP2017

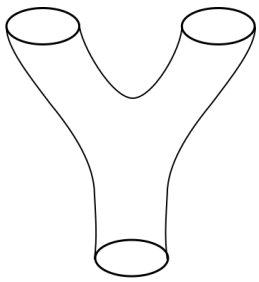
Book of abstracts

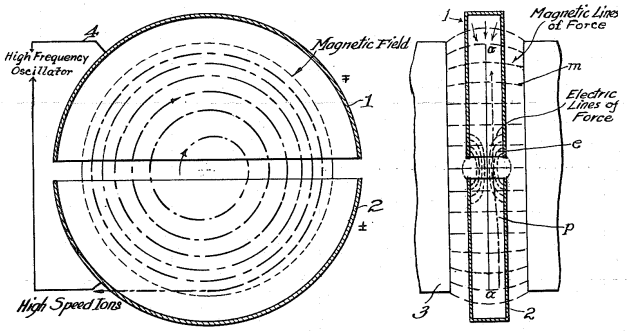












Paris, 9-13 July 2017

Welcome to CCP2017

We are delighted to< welcome you to the XXIXth IUPAP Conference in Computational Physics at the Campus Jussieu, UPMC, ideally located in the center of Paris. Attendees can look forward to three and a half days of exciting and stimulating talks covering all fields of computational physics. These include nine plenary lectures in the main auditorium of the conference center. The Young Scientific Prize 2017 of the IUPAP C20 commission will be awarded on this occasion to Glen Evenbly. The conference is followed by one half-day spin-off meeting on the history of simulation.

The IUPAP Conference in Computational Physics (CCP) is a series of conferences held annually under the auspices of the International Union of Pure and Applied Physics (IUPAP) on the basis of endorsement by its Commission on Computational Physics (C20). The application of computation is ever increasing and far-reaching in all aspects of science and so in physics. It is a major building block of the modern day science. This 29th edition will present the latest techniques and discoveries to the computational scientists working in various branches in physics and closely related areas.

The proceedings of the conference will be published in the open access Journal of Physics: Conference Series (JPCS) from IOPscience. The book of abstract can be downloaded for free from the conference website.

CCP2017 is grateful to its local host UPMC and to the sponsoring institutions for their support and to all participants for contributing to a rich scientific program.

Scientific Topics

Education

Astrophysics

Nuclear, Particle and Fields Physics

Atomic, Molecular and Optical Physics

Quantum Many Body Physics

Classical Statistical Mechanics

Fluid Dynamics: from Macro- to Nano-fluidics

Chemical Physics

Soft Matter and Biophysics

Materials Science

Energy Storage and Production

Geosciences and Climate Modeling

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Monday 10.07

Plenary session – Auditorium (PLN-1)
Chair : S. Baroni

08:50-09:00	Welcome *A. M. Saitta, R. Spezia, R. Vuilleumier (UPMC)*
09:00-10:00	**Plenary** - Materials discovery and scientific design by computation: what does it take? *G. Galli (U. of Chicago)*
10:00-11:00	**Plenary** - Multiscale Lattice Boltzmann Simulations at the Physics-Biology Interface *S. Succi (CNR, Rome)*
Coffee break	
11:30-12:30	**Plenary** - The Quantum Way of Doing Computations *R. Blatt (Universität Innsbruck)*

Lunch

Materials Sciences – Room 108/44-45 (MS-1)
Chair: G. Galli

14:00-14:40	**Keynote** - Car and Parrinello meet Green and Kubo: simulating heat transport from ab initio equilibrium molecular dynamics. *S. Baroni (SISSA, Trieste)*
14:40-15:05	Phonon-phonon interactions in semiconductors and in bismuth, and their effect on the electronic and thermal transport. *N. Vast (Laboratoire des Solides Irradiés)*
15:05-15:30	Quantum model of optical properties and thermal emission of superradiant electronic excitations. *A. Vasanelli (CNRS, Univ. Paris 7)*
Coffee break	
16:00-16:25	Quantum effect on site preference and diffusion of interstitial hydrogen in face-centered cubic metals. *H. Kimizuka (Osaka University)*
16:25-16:50	Structural and dynamical properties of methane hydrate under high pressure via Raman spectroscopy and first-principles molecular dynamics including nuclear quantum effects. *S. Schaack (INSP, UPMC)*
16:50-17:15	Regulation of structure and thermoelectric properties of the smallest SnTe nanowires via encapsulation within single-walled carbon nanotubes. *A. Vasylenko (Dept. Of Physics, Warwick)*
17:15-17:40	Multiscale modelling of nanoscale materials and electronic transport. *W. Wenzel (Karlsruhe Institute of Technology)*

Classical Statistical Mechanics – Room 105/44-54 (CSM-1)
Chair: S. Succi

14:00-14:40	**Keynote** - Scalable and efficient first-principles based Monte Carlo simulations on high performance computers *Y. W. Li (Oak Ridge National Laboratory)*
14:40-15:05	Wang-Landau algorithm with the control of accuracy *L. Shchur (Landau Institute for Theor. Phys.)*
15:05-15:30	Large deviations for equilibrium and non–equilibrium processes *A. Hartmann (Univ. of Oldenburg)*
Coffee break	
16:00-16:25	Computations of self-assembly of rod-like particles on a plane *Y. Tarasevich (Astrakhan State University)*
16:25-16:50	Vapor nucleation under extreme confinement. *S. Meloni (Univ. of Rome "Sapienza")*
16:50-17:15	Nucleation to percolation: crack growth in random spring ladder *P. Ray (The Institute of Mathematical Sciences)*

Chemical Physics – Room 106/44-45 (CP-1)
Chair: B. Peters

14:00-14:40	**Keynote** - Modelling Supramolecular Polymers *B. Sundaram (JNCASR, India)*
14:40-15:05	SFG spectroscopy of Silica/water interfaces by DFT-MD simulations *S. Pezzotti (LAMBE, Evry)*
15:05-15:30	Improving Solubility in Supercritical CO2: Theoretical Studies of CO2-philic Compounds and Solubilizers *F. Ingrosso (SRSMC, Nancy)*
Coffee break	
16:00-16:25	Simplifying calculations of IR and Raman spectra from DFT-based molecular dynamics simulations *D. R. Galimberti (LAMBE, Evry)*
16:25-16:50	Vibrational energy relaxation at water interfaces from ab initio molecular dynamics simulations *D. Lesnicki (University Mainz)*
16:50-17:15	All-trans, all-cis and mixed isomers of azobenzene star: A multiscale simulation study *M. Koch (Technische Universität Dresden)*
17:15-17:40	Hidden Beneath the Surface: Origin of the Observed Enantioselective Adsorption on PdGa(111) *D. Passerone (EMPA, Switzerland)*

Quantum Many Body Physics – Room 107/44-54 (QMB-1)
Chair: M. Casula

14:00-14:40	**Keynote** - Cluster multipole theory for anomalous Hall effect in antiferromagnets *R. Arita (RIKEN Center for Emergent Matter Science)*
14:40-15:05	Spin-Charge Coupling in Unconventional Superconductors: Insights from Diffusion Monte Carlo *A. Narayan (Materials Theory, ETH Zurich)*
15:05-15:30	Doping dependence of charge order in electron-doped cuprate superconductors *S. Feng (Beijing Normal University)*
Coffee break	
16:00-16:25	Carbon nanotubes as excitonic insulators *M. Rontani (CNR, Modena)*
16:25-16:50	Recent Advances in Thermally-Assisted-Occupation Density Functional Theory (TAO-DFT) *J.-D. Chai (National Taiwan University)*
16:50-17:15	Dephasing and disorder effects in the topological systems *X. C. Xie (Peking University)*
17:15-17:40	Nature of Quasi-Particle Excitations in the Spin-1/2 Square-Lattice Heisenberg Antiferromagnet *H. Shao (Boston University and Beijing Computational Science Research Center)*

Atomic, Molecular and Optical Physics
Room 109/44-54 (AMOP-1)
Chair: F. Werner

14:00 - 14:40	**Keynote** - Towards controlled description of correlated fermions: diagrammatic Monte Carlo for the Hubbard model. *E. Kozik (King's College London)*
14:40 - 15:05	C++QED: a framework for simulating open quantum dynamics – the first ten years *A. Vukics (Centre for Physics of the Hungarian Academy of Sciences)*
15:05 - 15:30	Numerical simulation of sympathetic cooling in radiofrequency ion traps for studies on antimatter *N. Sillitoe (Laboratoire Kastler Brossel)*
Coffee break	

Poster session – Patio, 18:00-20:00

Tuesday 11.07

Plenary session – Auditorium (PLN-2)
Chair : R. Vuilleumier

09:00-10:00	**Plenary** - Nuclear Physics as Precision Science *Ulf-G Meißner (Universität Bonn and Forschungszentrum Jülich)*
10:00-11:00	**Plenary** - Numerical Relativity in the Era of Multi-Messenger Astronomy *M. Campanelli (Rochester Institute of Technology)*
Coffee break	
11:30-12:30	**Plenary** - Multiscale characterization of macromolecular dynamics *C. Clementi (Rice University)*

Lunch

Materials Science – Room 108/44-45 (MS-2)
Chair: B. Sundaram

13:50-14:15	Absence of spin edge polarization of acenes in the long-chain limit M. Casula (CNRS, UPMC)
14:15-14:40	Accurate ground-state correlation energies within the RPA and beyond: Theory and applications to molecules and zeolites *D. Rocca (Laboratoire CRM2)*
14:40-15:05	Electronic and Structural Properties of K-doped NiO Mott-Insulator : Quantum Monte Carlo Study *H. Shin (Argonne National Laboratory)*
15:05-15:30	Development of a joint refinement model for the one-electron reduced density matrix using different data sets *S. Gueddida (CentraleSupélec Paris)*
Coffee break	
16:00-16:25	Interplay between morphology and properties of core-shell Fe@Au nanoparticles *M. Benoit (CEMES, Toulouse)*
16:25-16:50	UV-Visible Absorption Spectra of Silver Clusters from TDDFT Calculations *R. Schira (Institut Lumière Matière, Grenoble)*
16:50-17:15	On the coordination of the Zn(II) ion in bistriflimide-based Ionic Liquids: Structural and dynamics properties at varying nature of the cation *F. Sessa (Università di Roma "La Sapienza")*
17:15-17:40	Unraveling the Icosahedral geometry of a light lanthanoid ion in a protic ionic liquid: a combined Molecular Dynamics and EXAFS study *A. Serva (Università di Roma "La Sapienza")*

Classical Statistical Mechanics – Room 105/44-54 (CSM-2)
Chair: L. Shchur

13:50-14:15	Deep Learning for Fatigue Estimation on the Basis of Multimodal Human-Machine Interactions *N. Gordienko (National Technical University of Ukraine)*
14:15-14:40	Non-canonical spin glass of polyhedral spin models on quasi-regular lattices *T. Surungan (Hasanuddin University, Indonesia)*
14:40-15:05	Synchronisation of Conservative Parallel Discrete Event Simulations in Small World Network *L. Ziganurova (Science Center in Chernogolovka, Moscow)*
15:05-15:30	GPU accelerated population annealing algorithm and its application to first- and second-order phase transitions – *L. Barash (Landau Institute for Theoretical Physics)*
Coffee break	
16:00-16:25	Phase transitions in evolutionary space games *E. Burovski (State University Higher School of Economics, Moscow)*
16:25-16:50	Contour analysis of multi-affine nanostructure AZO thin films *S. Hosseinabadi (Islamic Azad University, Tehran, Iran)*
16:50 - 17:15	Melting transition of skyrmion lattice in a two-dimensional chiral magnet *Y. Nishikawa (The University of Tokyo)*
17:15 - 17:40	Effect of temperature specification on simulated ergodicity *R. Ocaya (University of the Free State, South Africa)*

Chemical Physics – Room 106/44-45 (CP-2)
Chair: G. Ciccotti

14:00 - 14:40	**Keynote** - Rare Events Methods, Reaction Coordinates, and Useful Rate Theories *B. Peters (University of California, Santa Barbara)*
14:40 - 15:05	Ab initio molecular dynamics simulations of RNA nucleotides in hydrothermal prebiotic environment *A. Pérez Villa (IMPMC, UPMC)*
15:05 - 15:30	Open Boundary / Grand-Canonical Adaptive Resolution Simulations of Ionic Liquids *C. Krekeler (Freie Universität Berlin)*
Coffee break	
16:00 - 16:25	On the dynamics through a conical intersection *F. Agostini (University Paris-Sud, University Paris-Saclay)*
16:25 - 16:50	Nuclear quantum effects in molecular dynamics simulations *H. Dammak (Centrale Supélec)*
16:50 - 17:15	Estimating thermodynamic expectations and free energies in expanded ensemble simulations: systematic variance reduction through conditioning *M. Athenes (CEA, France)*
17:15 - 17:40	Free energies of solvation and binding, and solvent positions around any molecule in few minutes by rigorous liquid state théories *M. Levesque (ENS, UPMC)*

Quantum Many Body Physics – Room 107/44-54 (QMB-2)
Chair: H.-Q. Lin

13:50-14:15	Ab initio approach to strong correlations in lanthanide compounds: from localized magnets to heavy-fermions. – *L. Pourovskii (Ecole Polytechnique)*
14:15-14:40	Simulations of electron energy loss spectra with turboEELS *O. Motornyi (Ecole Polytechnique)*
14:40-15:05	Controlled summation of diagrammatic series for the unitary Fermi gas: bold diagrammatic Monte Carlo, large-order asymptotics and conformal-Borel transformation – *F. Werner (Laboratoire Kastler Brossel, ENS)*
15:05-15:30	Towards exascale simulations of quantum superfluids far from equilibrium *P. Magierski (Warsaw University of Technology)*
Coffee break	
16:00-16:25	Assessing theoretical spectroscopy from novel first-principle approaches *S. Backes (Ecole Polytechnique)*
16:25-16:50	Off-Diagonal Expansion Quantum Monte Carlo *I. Hen (University of Southern California, Los Angeles)*

16:50-17:15	Dynamics of nuclear fission within the time-dependent generator coordinate method *D. Regnier (Institut de Physique Nucléaire d'Orsay)*
17:16-17:40	Connected Determinant Diagrammatic Monte Carlo: polynomial-time complexity thanks to the fermionic sign *R. Rossi (Laboratoire de Physique Statistique de l'ENS)*

Soft Matter and Biophysics – Room 109/44-54 (SMB-1)
Chair: C. Clementi

14:00-14:40	**Keynote** - Molecular simulations of membrane sensing and remodeling *G. Hummer (MPI Biophysics, Goethe Univ. Frankfurt)*
14:40-15:05	Electron Transfer in Organic and Biological Materials *A. Carof (University College London)*
15:05-15:30	Protein adaptation to high temperatures does not necessary require enhanced mechanical stability *G. Stirnemann (IBPC, Paris)*
Coffee break	
16:00-16:25	The challenge for Gram-negative bacteria: Towards in-silico screening of antibiotics for fast permeation through nanopores M. Ceccarelli (University of Cagliari, Italy)
16:25-16:50	Finding protein folding funnels in random networks M. Kikuchi (Osaka University)
16:50-17:15	Theoretical studies on stability and dynamics of protein complex by a coarse-grained model H. Nagao (Kanazawa University)
17:15-17:40	Weak Nanoscale Chaos And Anomalous Relaxation in DNA A. Mazur (IBPC, Paris)

Poster session – Patio, 18:00-19:30

Gala Dinner – La Coupole, 20:00-22:00

Wednesday 12.07

Plenary session – Auditorium (PLN-3)
Chair : J. Adler

09:00-10:00	**Plenary** - Potential Energy Surfaces and Berry Phases beyond the Born-Oppenheimer Approximation: A New Approach to Non-Aadiabatic Dynamics *E.K.U. Gross Max Planck Institute, Halle)*
10:00-11:00	**Plenary** - Theoretical Physics is More than Equations: The African School for Electronic Structure Methods and Applications *R. M. Martin (University of Illinois at Urbana Champaign, Stanford University)*
Coffee break	
11:30-12:30	**YSP2017 award** - Tensor Network Renormalization *Glen Brian Evenbly (University of Sherbrooke)*

Lunch

Materials Science – Room 108/44-45 (MS-3)
Chair: M. Lazzeri

14:15-14:40	Chemisorption of Hydroxides on Carbon and Boron Nitride Nanomaterials from Ab Initio Calculations *B. Grosjean (École Normale Supérieure, Paris)*
14:40-15:05	Multiscale Modeling of the Insertion and Diffusion of H-3 and Cl-36 in UNGG Graphite *Christoph Lechner (EDF R&D)*
15:05-15:30	Molecular dynamics modeling of graphite and graphene melting *N. Orekhov (Moscow Institute of Physics and Technology)*
Coffee break	
16:00-16:25	Atomistic Simulations of the Assembly of Large Gold Nanocrystals *J. Richardi (UPMC, Paris)*
16:25-16:50	On the oxidation state of titanium in titanium dioxide *S. Manzhos (National University of Singapore)*
16:50-17:15	Ab initio study of inorganic perovskites: towards the prediction of PbZr_1-x_Ti_x_O_3 (PZT) IR spectrum *Y. Peperstraete (Synchrotron SOLEIL)*
17:15-17:40	Study of the ferroelectric properties of epitaxially strained SrTaO2N by means of DFT all-electrons first principles calculations. *Roberto Alonso (Conicet, Argentina)*

Nuclear, Particle and Fields Physics – Room 105/44-54 (NPFP-1)
Chair: G. B. Evenbly

14:00-14:40	**Keynote** - Machine Learning from the proton structure to Higgs pair production at the LHC *J. Rojo (Vrije University, Amsterdam)*
14:40-15:05	Transformed Lattice Rules for Feynman Loop Integrals *E. de Doncker (Western Michigan University)*
15:05-15:30	ATLAS Track reconstruction at the energy frontier *A. Kastanas (KTH Royal Institute of Technology)*
Coffee break	
16:00-16:25	The new ATLAS Fast Calorimeter Simulation *H. Ahmed (University of Edinburgh)*
16:25-16:50	Statistical and systematic errors in the analysis of multiple datasets *O. Selyugin (Universite de Liege)*
16:50-17:15	Novel methods in track-based alignment to correct for time-dependent distortions of the ATLAS Inner Detector *Oscar Estrada (CERN)*
17:15-17:40	Primary Vertex Reconstruction with the ATLAS experiment *D. Casper (CERN)*

Classical Statistical Mechanics – Room 107/44-54 (CSM-3)
Chair: E. Trizac

13:50-14:15	Random Field Ising Model with Conserved Kinetics: Super-Universality Violation, Logarithmic Growth Law and the Generalized Tomita Sum Rule *V. Banerjee (Indian Institute of Technology, Delhi)*
14:15-14:40	Improving and testing the population annealing Monte Carlo algorithm *Martin Weigel (Coventry University)*

Quantum Many Body Physics – Room 107/44-54 (QMB-3)
Chair: T. Xiang

14:40-15:05	Coupled Electron-Ion Monte Carlo study of hydrogen under extreme conditions *Markus Holzmann (CNRS, Université Grenoble-Alpes)*
15:05-15:30	Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of multireference perturbation theory *Y. Garniron (IRSAMC)*
Coffee break	

16:00-16:25	Importance of correlation effects for theoretical description of pressure induced electronic transitions: IMT, ETT, CLC. *I. Abrikosov (Linköping University, Sweden)*
16:25-16:50	Proposal of a new fully uncontracted multi-reference perturbation theory *E. Giner (MPI for Solid State Research)*
16:50-17:15	Diagrammatic extensions of DMFT: Nonlocal interactions and nonlocal corrélations *E. van Loon (Radboud University, Nijmegen)*

Soft Matter and Biophysics – Room 109/44-54 (SMB-2)
Chair: G. Hummer

14:15-14:40	Conformational dynamics of the human Guanylate binding protein 1 from Hamiltonian replica exchange MD simulations and FRET experiments *B. Barz (Jülich Research Centre, University Düsseldorf)*
14:40-15:05	Mesoscale Hydrodynamic Simulation of Microswimmers *R. Winkler (Forschungszentrum)*
15:05-15:30	Monte Carlo simulation for pattern formation of run-and-tumble chemotactic bacteria *S. Yasuda (University of Hyogo)*
Coffee break	
16:00-16:25	Transition to network synchronization in neuronal cultures: modelling the activity bursts with an adaptive 2D dynamical model *P. Monceau (Université Paris-Diderot)*
16:25-16:50	Viscoelastic hydrodynamic interactions and anomalous CM diffusion in polymer melts: influence of thermostat and simulation box *H. Meyer (Institut Charles Sadron)*

FLuid dynamics : from macro to nano – Room 109/44-54 (FD-1)
Chair: D. Passerone

16:50-17:15	Numerical investigation on spreading behavior of falling droplet on inclined surface *S. Pati (National Institute of Technology Silchar, India)*
17:15 - 17:40	Solidification of a simple liquid near wall in high-speed lubrication flows *Shugo Yasuda (University of Hyogo)*

Energy Storage and Production – Room 106/44-45 (ESP-1)
Chair: R. Spezia

14:00 - 14:40	**Keynote** - Understanding Ionic liquids role in energy application from calculations *B. Kirchner (University of Bonn)*
14:40 - 15:05	Modelling Nanoporous Graphene Based Supercapacitors *T. Méndez Morales (Maison de la Simulation – CEA)*
15:05 - 15:30	Confinement Effects on an Electron Transfer Reaction in Nanoporous Carbon Electrodes *Z. LI (CEA – UPMC – RS2E)*
Coffee break	

Chemical Physics – Room 106/44-45 (CP-3)
Chair: M. Salanne

16:00-16:25	Analysis of local bond-orientational order for liquid gallium at ambient pressure *T.-M. Wu (National Chiao-Tung University)*
16:25-16:50	Interlayer binding of bilayer blue phosphorus: quantum Monte Carlo study *J. Ahn (Konkuk University)*

Thursday 13.07 Morning

Materials Science – Room 108/44-45 (MS-4)
Chair: M.-L. Bocquet

09:00-09:40	**Keynote** - Embedded many-body perturbation theories for organic optoelectronics *X. Blase (Institut Néel)*
09:40-10:05	Optical properties of single-molecule junctions *Herve Bulou (IPCM, Strasbourg)*
10:05-10:30	On screening in organic semi conductors *S. Gueddida (CentraleSupélec Paris)*
Coffee break	
11:00-11:25	Buckled monolayer of GaAs under transverse electric field *B. Prasad (National Institute of Technology, Surat)*
11:25-11:50	Numerical analysis of Brillouin zone integration methods *A. Levitt (MATHERIALS)*

FLuid dynamics : from macro to nano – Room 109/44-54 (FD-2)
Chair: B. Rotenberg

09:00-09:40	**Keynote** - Hydration friction in nano-confinement: from bulk via interfacial to dry friction *R. Netz (TU Berlin)*
09:40-10:05	Molecular dynamics simulations of diffusio-osmotic flow driven by chemical potential gradient *H. Yoshida (ENS, Paris, Toyota Central R&D Labs., Inc.)*
10:05-10:30	Multiscale modelling of ion adsorption and electrokinetic phenomena in porous oxides. *J.-F. Dufrêche (ICSM, Marcoule)*
Coffee break	
11:00-11:25	Transient hydrodynamic finite size effects in simulations under periodic boundary conditions *A. Asta (Phenix, UPMC)*
11:25-11:50	Design criteria for underwater superhydrophobicity: a rare-event molecular dynamics study *Matteo Amabili (University of Rome "La Sapienza")*

Geosciences and Climate Modelling – Room 105/44-54 (Geo-1)
Chair: A. Vasanelli

09:00-09:40	**Keynote** - Towards high-resolution climate models *C. Schär, (ETH Zurich)*
09:40-10:05	Bridging the Scale Hierarchy Problem in Biogeochemical Models *F. Paparella (New York University Abu Dhabi)*
10:05-10:30	Hierarchies of complexity in Earth System Modeling *V. Balaji (Princeton University)*
Coffee Break	
11:00-11:25	Importance of a fully anharmonic treatment of equilibrium isotope fractionation properties of dissolved ionic species as evidenced by Li+(aq) *M. Méheut (Géosciences Environnement Toulouse)*
11:25-11:50	Investigating the properties of silicate and carbonate melts at Earth's mantle conditions by molecular dynamics simulation *Nicolas Sator (UPMC, Paris)*

Quantum Many Body Physics – Room 107/44-54 (QMB-4)

Chair: S. Biermann

09:00-09:40	**Keynote** - Gapless Spin-Liquid Ground State in the S=1/2 Kagome Antiferromagnet *T. Xiang (Chinese Academy)*
09:40-10:05	Quantum spin phases emerged from the interplay between strong correlation and spin-orbital coupling *J. Li (Nanjing University)*
10:05 - 10:30	Short-time quantum critical dynamics for Ising model in a transverse field *D. Yao, (Sun Yat-Sen University)*
Coffee break	

Energy Storage and Production – Room 107/44-54 (ESP-2)

Chair: B. Kirchner

11:00-11:25	Proton Mobility in Protic Ionic Liquids: New Results from Theoretical Calculations *E. Bodo (University of Rome "La Sapienza")*
11:25 - 11:50	Comparative Density Functional Theory - Density Functional Tight Binding study of fullerene derivatives: effects of addends, buckyball size, and crystallinity on properties affecting solar cell functionality *S. Manzhos (National University of Singapore)*

Astrophysics – Room 106/44-45 (Astro)

Chair: P. Ray

09:00-09:40	**Keynote** - Gravitational waves: The new frontier of astrophysics *P. Ajith (International Centre for Theoretical Sciences)*
09:40-10:05	Simulation of magnetorotational processes in core-collapsed supernovae *S. Moiseenko (Space Research Institute, Russia)*
10:05 - 10:30	Modeling of Fragmentation and Density Stratification in the Process of Shock Interaction with Molecular Clouds on Grids with Very Large Resolution *B. Rybakin (Lomonosov Moscow State)*
Coffee break	

Education – Room 106/44-45 (Educ)

Chair: R. Martin

11:00-11:25	Groundstates of liquid crystals with colloids: a project for undergraduate students *J. Adler (Technion - Israel Institute of Technology)*
11:25 - 11:50	Toolkit-based approach to undergraduate training in molecular dynamics *Richard Ocaya (University of the Free State)*
11:50 - 12:15	Time evolution of the unstable soliton solution for dust acoustic waves with trapped électrons *S. Phibanchon (Faculty of Education, Burapha Univeristy)*

Concluding Remarks – Room 108/44-45

12:30-12:45	Conclusions *A. M. Saitta, R. Spezia, R. Vuilleumier*

Thursday 13.07 Afternoon : Spin-off meeting on the history of simulation

Amphitheater Charpak

Chair : D. Borgis and E. Vanden-Eijnden

14:00-14:45	The Birth, Rise and Triumph of Molecular Dynamics *J.-P. Hansen (Cambridge – UPMC)*
14 :45-15 :30	Electronic Structure Computation from the first years after the advent of quantum mechanics to challenges today *R. Martin (University of Illinois)*
Coffee break	
16 :00-16 :45	How has Molecular Simulation contributed to the dream of Theoretical physics? An attempt at an historical reconstruction *G. Ciccotti (Univerity of Rome « La Sapienza »)*
16 :45-17 :15	Round Table *D. Borgis (Maison de la simulation – ENS), E. Vanden-Eijnden (New York University)*

List of posters

Astrophysics

P1. Propagation of Dust-Ion Acoustic (DIA) waves in multi-species plasma with Cairn's distributed electrons, quantum effects in inertia less electrons and ions
Kalita Bhaben Chandra, Das Samiran

P2. Investigation of dust ion acoustic (DIA) solitons in multicomponent plasma with relativistic ions and Cairns distributed électrons
Das Samiran, B.C. Kalita

P3 The role of the order of perturbation and its determination in the process of enforcing discrete Korteweg-de-Vries solitons to modified Korte-de-Vries solitons as means of continuum hypothesis in a multi component dusty plasma
Kalita Bhaben

P4 Complexity Cmp and Time's Arrow
Rajilic Zoran

Nuclear, Particle and Fields Physics

P5. Computational studying energy and spectral parameters of hadronic (pionic) atoms with account of the strong pion-nuclear interaction
Dubrovskaya Yuliya

P6. Computational studying the hyperfine and electroweak interaction and parity violation in heavy finite Fermi-systems: Advanced Code
Khetselius Olga

P7. Confinement and Chiral Phase Transition in Dual QCD Formulation.
Punetha Garima

P8. SU(3) Dual QCD formulation and quark-hadron phase transition
Punetha Garima

P9. Implications of general lepton mass matrices in the standard model for Neutrinoless Double Beta Decay parameter m_{ee}
Sharma Samandeep

Atomic, Molecular and Optical Physics

P10. Advanced computational approach to studying Rydberg and autoionization resonances in spectra of heavy lanthanides and actinides
Ternovsky Valentin

P11. Advanced computational approach to nonlinear dynamics of laser systems with elements of a chaos
Ternovsky Valentin

P12. Advanced relativistic model potential approach to computing the radiation transition characteristics for atoms and multicharged ions
Buyadzhi Vasily

P13. Advanced computational approach in electron-collisional spectroscopy of atoms and multicharged ions in plasmas
Buyadzhi Vasily

P14. Cooperative laser electron-gamma-nuclear phenomena in dynamics and spectroscopy of molecules: Advanced Computational Code
Glushkov Alexander

P15. New relativistic computational energy approach to heavy Fermi-systems in a super strong field: AC Stark and multi-photon resonances
Glushkov Alexander

P16. Advanced computational code to « shake-up » and NEET effects in laser electron-gamma-nuclear spectroscopy of atoms and ions
Khetselius Olga

P17. Modulation of Intense Femtosecond Laser Pulse by a strong magnetic field
Shu Xiaofang

P18. Superexchange Interatomic Coulombic decay by Fano-ADC-Stieltjes method
Votavov· Petra

P19. Projectile Charge Effect on Electron and Positron Impact Single Ionization Cross Sections of Plasma Relevant Molecular Targets
Singh Prithvi

P20. Computer simulation of the interaction of fullerene with nanographene
Stelmakh Vasiliy

P21. Ab- initio calculation of the electronic gap, the refractif index of (PbTe), (SrTe) and Lead strontium telluride alloys (Pb1-xSrxTe).
Sifi Chahra, Chouit Fairouz, Sifi Chahra

Quantum Many Body Physics

P22. Quatum phase transition in a three-dimensional dimerized Heisenberg model on a corundum lattice
Miyahara Shin

P23. Enhancement of superconducting correlations by charge and spin ordering in coupled electron and spin systems
Farkasovsky Pavol

P24. Quantum Monte Carlo calculations of elastic properties of one-dimensional carbon chain
Hong Iuegyun

P25. Determination of energies dan wave functions of a quantum many-body system by the finite difference time domain (FDTD) with the Hartree Fock (HF) approximation
Sudiarta I Wayan

P26 Prediction of electronic and optical properties of ZnAl2Te4 defect chalcopyrite semiconductor: an ab-initio study
Tripathy Susanta Kumar

Classical Statistical Mechanics

P27. Coarse analysis of non-equilibrium collective phenomena: Bifurcation analysis of the optimal velocity model using diffusion maps
Sugiyama Yuki

P28. Monte Carlo Study of a Three States Spin Model
Luque Luciana

P29 Study of the kinetic effects in homogeneous and heterogeneous bubble cavitation via atomistic simulations
Marchio Sara

P30. The SAPBC method on local, non-cluster updates algorithms of Monte Carlo simulation: A study on more convergence of spin correlation at critical temperature.
Najafi Amin

P31. Fast customization of the Wang Landau parallel algorithm for the different lattices
Arman Kussainov

P32. Mean squared displacement of dust particles in 2-dimensional strongly coupled Yukawa liquids exposed to an external magnetic field
Masheyeva Ranna

Fluid Dynamics: from Macro- to Nano- fluidics

P33. Multiple eigen-modes of Rayleigh-Taylor instability observed for a smoothly varying density fluid interface
Yu Chengxin

P34. Ion acoustic solitary waves with high relativistic thermal ions and non-thermal electrons and thermal positrons in plasma
Das Ranjan

P35. Computational Model Of Calcium And IP3 Dynamics: A Finite Difference Method Approach
Singh Nisha

Chemical Physics

P36. DFT Computational and Spectroscopic Investigations on The Cyanide Bridged Heteronuclear Polymeric Complex: [Cd(N-Meim)2Ni(μ-CN)4]n
Kurkcuoglu Gunes Suheyla

P37 High performance and low complexity algorithm for MP2 calculations in solids
Schäfer Tobias

P38. Statistical vs non-statistical effects and the importance of the activation method in unimolecular fragmentation of peptides via chemical dynamics simulations
Macaluso Veronica

P39. Fully quantum description of the Zundel ion: combining variational quantum Monte Carlo with path integral Langevin dynamics
Mouhat Félix

P40. Molecular, vibrational, electronic structure and nonlinear optical properties of 1-ethylimidazole
Kurkcuoglu Gunes Suheyla

P41 Experimental and Computational Study on Photoreaction of Flutamide and Its Cyano Analogue
Fukuyoshi Shuichi

P42 Application of order-N first-principles DFT calculations with temperature controlled molecular dynamics to biomolecular system
Otsuka Takao

P43 A theoretical study on the molecular structure, vibrational (FT-IR and Raman) spectra and electronic transition energies of cyanide-bridged heteronuclear polymeric complex of 1-ethylimidazole: [Cu(etim)4Pd(μ-CN)4]n
Kurkcuoglu Gunes Suheyla

P44. Calcium Oxalate Polyhydrate morphologies from first principles
Debroise Théau

Soft Matter and Biophysics

P45. Solvation free energy in protein docking process: a molecular dynamics study
Mizukami Taku

P46 Study of coupled oscillators' locking pattern on complex networks
Kim Junhyeok

P47. Computational studies on cyclic imide formation mechanism of glutamic acid residues catalyzed by two water molecules
Nakayoshi Tomoki

P48. Free energy profiles of lipid translocation across mixed lipid bilayers: a molecular dynamics study
Saito Hiroaki

P49 Prediction of three-dimensional structures of histone deacetylase 1 complexed with romidepsin and its analog
Oda Akifumi

P50. Effect of the Arg456His mutation on the three-dimensional structure of cytochrome P450 1A2 predicted by molecular dynamics simulations
Watanabe Yurie

P51. Molecular dynamics study of interaction between PACAP (6'?38') and N-terminal extracellular domain of the human splice variant hPAC1-R-short aiming at development of neuropathic pain medicine
Watanabe Yurie

P52. Structural differences of the ligand binding pockets between estrogen receptor alpha and beta
Kato Koichi

P53. Fickian Yet Non-Gaussian Behaviour: A Dominant Role of the Intermittent Dynamics
Acharya Sayantan, Maitra Bhattacharyya Sarika

Materials Science

P54. DFT study of the vibrational and electronic properties of InAs nanowires
Cruz-Irisson Miguel

P55. Modelling of the quantum confinement effects on the optical properties of GaSb nanowires
Cruz-Irisson Miguel

P56. Metal-porphyrin-like graphenes for selective ammonia capture
Yang Hyungmo

P57 Structural Rietveld refinement and vibrational study of ZnxCo1-xFeO4 spinel ferrites
Rais Abdelmajid, Addou Ahmed

P58. I-V Characteristics of Graphene Nanoribbon/h-BN Heterojunctions
Tomiya Mitsuyoshi

P59. The driving force for the charge ordering in the nickelates
Mahadevan Priya

P60. Effect of p- and n-type dopant on optoelectronic properties of 2D-HfS2
Singh Deobrat

P61. Mathematical model of novel concept of optical image registration in wide spectral range by piezoelectric microresonators
Pigarev Aleksey

P62. The thermodynamic properties and bonding feature of the some B2 rare-earth intermetallic compounds: first principal study
Abdessamad Sekkal

P63. Crystal Structures, Electronic, Vibrational and Optical Properties of few Single Monolayer of SnH, *Kumar Vipin*

P64. Structural, electronic and magnetic properties of GdFeSi : DFT+U study
Dine Khaled

P65. Computational Studies of The Development of GLI-associated oncogene inhibitory Synthetics
Rifai Yusnita

P66. Band Gap Tuning of Alumina by Surface Adsorption of II Group Elements: a DFT Study
Janki Shah

P67. Development of Reliable Interaction Potential for and Results of Molecular Dynamics Simulations of ZrO2 Film Growth
Houska Jiri

P68. Band Gap of BN co-doped Graphene, first-principles investigation.
Nascimento Regiane

P69. High Pressure Structural Phase Transition in NdX (X=P, As, Sb): A Density Functional Theory Study
Singh Sanjay

P70. The Effects of Vacancy-Defect, Adsorbent and Li Dopant on Electronic and Magnetic Attributes of MoO3 (010) Bilayer: A First-Principles Study
Mansouri Masoud

P71. First Principle Study on the Structure, Electronic and Optical Properties of MoS2 /AlN Hybrid Bilayer
Kumar Vipin, Roy Debesh

P72. High-throughput screening of carbon-capturing materials with ab initio and thermodynamic calculation
Bae Hyeonhu

P73. First-Principles Approach of the Structural, Electronic and Dynamical Properties of SixGe(1-x) (0 ? x ? 1), SiC, GaX (with X = P, As, Sb): A Study of the Hybrid Functionals Performance.
Lafond Fabien

P74. Hard-Sphere Melting and Crystallization with Modern Hybrid Algorithms
Isobe Masaharu

Energy Storage and Production

P75. Investigation of electrode passivation phenomenon in Li-O2 batteries by means of macrokinetical modeling of RRDE experiments.
Sergeev Artem

P76. Strain Induced Modulation of 2D Transition Metal Dichalcogenides Homo and Heterostructure: Prediction from Computational Approach
Shivam Kansara

P77. Molecular simulation of aqueous electrolytes in nanoporous carbons: Blue Energy and water desalination
Ganfoud Nidhal

Geosciences and Climate Modeling

P78. New non-linear computational approach to analysis, modelling and prediction of chaotic variability of atmospheric radioactive radon 222Rn concentration in atmosphere environment
Buyadzhi Vasily

P79 New computational approach to modelling dynamics of air ventilation and forecasting pollutant concentrations temporal dynamics for city's atmosphere
Khetselius Olga

P80. New computational approach to the Earth atmosphere circulation and angle momentum balance modelling: Atmospheric circulation, teleconnection and radio-waveguides
Glushkov Alexander

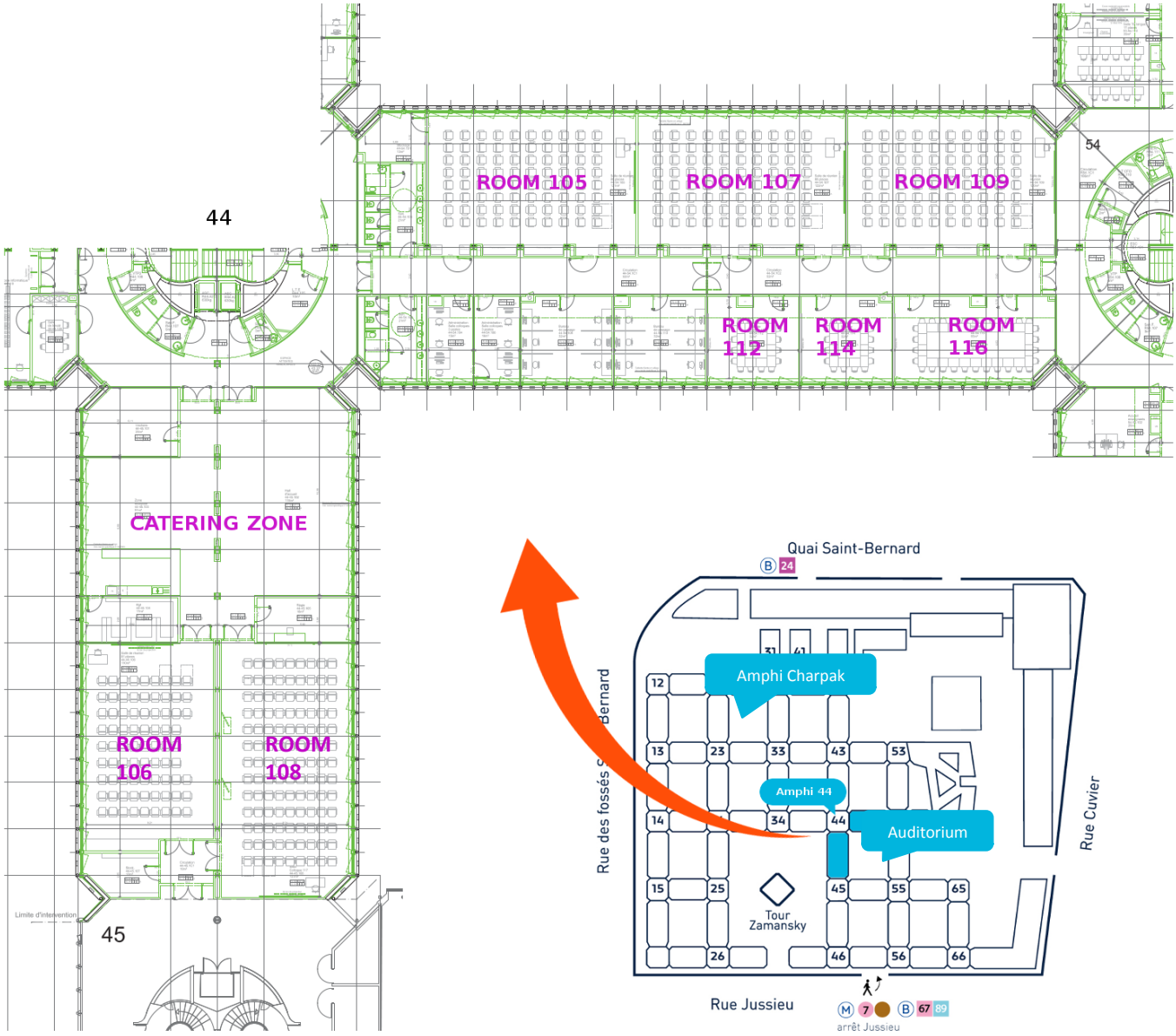
P81. Distribution of barchan dunes using a lattice model
Katsuki Atsunari

P82. A Mathematical Model for Solar and Anthropogenic Forcing of Global Climate
Tarafder Rajashik

P83. Direct simulation of outdoor blast waves
Lardjane Nicolas

Education

P84. Complex approach to the formation of ideas about the phenomenon of dynamic chaos for university students
Imanbayeva Akmaral



Auditorium

Plenary sessions, Morning coffee breaks

Patio 44-54

Welcome, Poster session, Lunch boxes, Afternoon coffee breaks

Rooms 106/44-45, 108/44-45, 105/44-54, 107/44-54, 109/44-54, Catering zone

Parallel sessions, Afternoon coffee breaks

Amphitheater Charpak

Thursday afternoon spin-off meeting on the history of simulation

Sunday 09.07	17:00-20:00	Patio	**Registration**
Monday 10.07	08:50-09:00	Auditorium	**Welcome**
	09:00-10:00	Auditorium	**Plenary Lecture** Materials discovery and scientific design by computation: what does it take? *G. Galli (U. of Chicago)*
	10:00-11:00	Auditorium	**Plenary Lecture** Multiscale Lattice Boltzmann Simulations at the Physics-Biology Interface *S. Succi (CNR, Rome)*
	11:00-11:30	Hall	**Coffee Break**
	11:30-12:30	Auditorium	**Plenary Lecture** The Quantum Way of Doing Computations *R. Blatt (Universität Innsbruck)*
	12:30-14:00	Patio	**Lunch**
	14:00-15:30	Conference center	**Parallel Sessions**
	15:30-16:00	Catering zone Patio	**Coffee Break**
	16:00-17:40	Conference center	**Parallel Sessions**
	18:00-20:00	Patio	**Poster session**
Tuesday 11.07	09:00-10:00	Auditorium	**Plenary Lecture** Nuclear Physics as Precision Science *Ulf-G Meißner (Universität Bonn and Forschungszentrum Jülich)*
	10:00-11:00	Auditorium	**Plenary Lecture** Numerical Relativity in the Era of Multi-Messenger Astronomy *M. Campanelli (Rochester Institute of Technology)*
	11:00-11:30	Hall	**Coffee Break**
	11:30-12:30	Auditorium	**Plenary Lecture** Multiscale characterization of macromolecular dynamics *C. Clementi (Rice University)*
	12:30-13:50	Patio	**Lunch**
	13:50-15:30	Conference center	**Parallel Sessions**
	15:30-16:00	Catering zone Patio	**Coffee Break**
	16:00-17:40	Conference center	**Parallel Sessions**
	18:00-19:30	Patio	**Poster session**
	20:00-22:00	La Coupole	**Gala dinner**
Wednesday 12.07	09:00-10:00	Auditorium	**Plenary Lecture** Potential Energy Surfaces and Berry Phases beyond the Born-Oppenheimer Approximation: A New Approach to Non-Aadiabatic Dynamics *E.K.U. Gross Max Planck Institute, Halle)*
	10:00-11:00	Auditorium	**Plenary Lecture** Theoretical Physics is More than Equations: The African School for Electronic Structure Methods and Applications *R. M. Martin (University of Illinois at Urbana Champaign, Stanford University)*
	11:00-11:30	Hall	**Coffee Break**
	11:30-12:30	Auditorium	**YSP2017 Award Ceremony** Tensor Network Renormalization *Glen Brian Evenbly (University of Sherbrooke)*
	12:30-13:50	Patio	**Lunch**
	13:50-15:30	Conference center	**Parallel Sessions**
	15:30-16:00	Catering zone Patio	**Coffee Break**
	16:00-17:40	Conference center	**Parallel Sessions**
Thursday 13.07	09:00-10:30	Conference center	**Parallel Sessions**
	10:30-11:00	Catering zone Patio	**Coffee Break**
	11:00-12:15	Conference center	**Parallel Sessions**
	12:30-12-45	Room 108/44-45	**Concluding Remarks**
	12:45-14:00	Patio	**Lunch**
	14:00-17:15	Amphi. Charpak	**Spin-off meeting on the history of simulations**

Table of contents

Plenary

The Quantum Way of Doing Computations

Rainer Blatt *† [1,2]

[1] Institute for Experimental Physics, University of Innsbruck – Technikerstrasse 25, A-6020 Innsbruck, Austria
[2] Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences – Otto-Hittmair-Platz 1, A-6020 Innsbruck, Austria

Since the mid-nineties of the 20th century, it became apparent that one of the centuries' most important technological inventions, computers in general and many of their applications could possibly be further enhanced by using operations based on quantum physics. This is timely since the classical roadmap for the development of computational devices, commonly known as Moore's law, will cease to be applicable within the next decade. This is due to the ever-smaller sizes of the electronic components that will enter the realm of quantum physics. Computations, whether they happen in our heads or with any computational device, always rely on real physical devices and processes. Data input, data representation in a memory, data manipulation using algorithms and finally, data output require physical realizations with devices and practical procedures. Building a quantum computer then requires the implementation of quantum bits (qubits) as storage sites for quantum information, quantum registers and quantum gates for data handling and processing as well as the development of quantum algorithms.

In this talk, the basic functional principle of a quantum computer will be reviewed. It will be shown how strings of trapped ions can be used to build a quantum information processor and how basic computations can be performed using quantum techniques. In particular, the quantum way of doing computations will be illustrated with analog and digital quantum simulations, which range from the simulation of quantum many-body spin systems over open quantum systems to the quantum simulation of a lattice gauge theory.

*Speaker
†Corresponding author: Rainer.Blatt@uibk.ac.at

Numerical Relativity in the Era of Multi-Messenger Astronomy

Manuela Campanelli *† [1]

[1] Rochester Institute of Technology – United States

The recent discovery of gravitational waves by Advanced LIGO ushered in a new kind of astronomy, one potentially integrating its findings with those obtained from electromagnetic and/or neutrino observations. Multi-messenger astronomy promises to revolutionize our understanding of the universe by providing dramatically contrasting views of the same objects. To understand this unprecedented wealth of observational evidence, computer intensive theoretical calculations of the Einstein field equations, coupled with the equations of magneto-hydrodynamics, are required in order to link data with underlying physics. In this talk, I will provide a review on the recent progress in this exciting field of computational astrophysics. With Advanced LIGO now fully operational and the detection of additional gravitational wave events imminent, we expect that there will be a surge in the number of researchers interested in performing simulations of compact binary mergers.

*Speaker

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Multiscale characterization of macromolecular dynamics

Cecilia Clementi *† [1]

[1] Rice University – United States

Macromolecular systems are central to biological processes. The complete characterization of the thermodynamic and kinetic of high dimensional dynamical systems such as large protein complexes still presents significant challenges. These processes involve the interplay of multiple length- and time-scales, and their understanding requires the development of new techniques at the interface of physics, mathematics, biology, computer science, and chemistry. We will discuss our attempts to tackle these points systematically, and recent applications to specific systems.

*Speaker
†Corresponding author: cecilia@rice.edu

Tensor Network Renormalization

Glen Evenbly *† [1]

[1] University of Sherbrooke – Canada

I will describe how to generate a proper RG flow for Euclidean path integrals of quantum systems on the lattice using a tensor network formalism. This approach, called tensor network renormalization (TNR), recovers scale-invariance for quantum systems at a critical point, and can be used to implement local scale transformations corresponding to lattice version of conformal maps. Applications of TNR towards the study of many-body systems, especially those at a critical point, and its relationship to tensor network ansatz will be discussed.

*Speaker
†Corresponding author: Glen.Brian.Evenbly@USherbrooke.ca

Materials discovery and scientific design by computation: what does it take?

Giulia Galli *† [1]

[1] Institute for Molecular Engineering, University of Chicago – United States

Substantial progress has been made in the last three decades in understanding and predicting the fundamental properties of materials and molecular systems from first principles, employing electronic structure methods and atomistic simulations. Using specific examples, I will discuss some of the major challenges involved in enabling scientific discoveries by computation; in particular I will touch upon theoretical validation; and collection, verification and use of data generated by simulations. I will also discuss some of the theoretical and algorithmic advances required to broaden the scope of properties accessible by current ab initio simulations.

*Speaker
†Corresponding author: gagalli@uchicago.edu

Potential Energy Surfaces and Berry Phases beyond the Born-Oppenheimer Approximation: A New Approach to Non-Aadiabatic Dynamics

E.K.U. Gross * [1]

[1] Max Planck Institute of Microstructure Physics (MPI-Halle) – Weinberg 2 06120 Halle (Saale), Germany

Some of the most fascinating phenomena in Chemistry and Physics, such as the process of vision, exciton dynamics in photovoltaic systems, as well as phonon-driven superconductivity occur in the regime where the non-adiabatic coupling of electronic and nuclear motion is essential. To tackle such situations one has to face the full Hamiltonian of the complete system of electrons and nuclei. We deduce an exact factorization [1] of the full electron-nuclear wavefunction into a purely nuclear part and a many-electron wavefunction which parametrically depends on the nuclear configuration and which has the meaning of a conditional probability amplitude. The equations of motion for these wavefunctions lead to a unique definition of *exact* potential energy surfaces as well as *exact* geometric phases, both in the time-dependent and in the static case. We discuss a case where the exact Berry phase vanishes although there is a non-trivial Berry phase for the same system in Born-Oppenheimer approximation [2], implying that in this particular case the Born-Oppenheimer Berry phase is an artifact. In the time-domain, whenever there is a splitting of the nuclear wavepacket in the vicinity of an avoided crossing, the exact time-dependent surface shows a nearly discontinuous step [3]. This makes the classical force on the nuclei jump from one to another adiabatic surface, reminiscent of Tully surface hopping algorithms. Based on this observation, we propose novel mixed-quantum-classical algorithms whose unique feature is that the trajectories are coupled. Without recourse to Tully surface hopping and without any added decoherence correction, the new algorithm provides a rather accurate, (much improved over surface hopping) description of decoherence.[4] This is demonstrated for the photo-induced ring opening of oxirane [5] (see figure). Finally, we present a multi-component density functional theory [6] that provides an avenue to make the fully coupled electron-nuclear system tractable for very large systems.

[1] A. Abedi, N.T. Maitra, E.K.U. Gross, Phys. Rev. Lett. 105, 123002 (2010).
[2] S.K. Min, A. Abedi, K.S. Kim, E.K.U. Gross, Phys. Rev. Lett. 113, 263004 (2014).
[3] A. Abedi, F. Agostini, Y. Suzuki, E.K.U. Gross, Phys. Rev. Lett. 110, 263001 (2013).
[4] S.K. Min, F. Agostini, E.K.U. Gross, Phys. Rev. Lett. 115, 073001 (2015).
[5] F. Agostini, S.K. Min, I. Tavernelli, E.K.U. Gross, J. Phys. Chem. Letters (2017).
[6] R. Requist, E.K.U. Gross, Phys. Rev. Lett. 117, 193001 (2016).

*Speaker

Theoretical Physics is More than Equations: The African School for Electronic Structure Methods and Applications

Richard M. Martin * [1,2]

[1] University of Illinois at Urbana Champaign (UIUC) – University of Illinois at Urbana-Champaign • Department of Physics Urbana, IL 61801-2302 webmaster@cs.illinois.edu, United States
[2] Stanford University – Stanford, California 94305, United States

Theoretical physics is an integral part of knowledge that belongs to the global community. Even though it is formulated in terms of fundamental equations, it is a human endeavor that benefits all people through technological and intellectual advances. Education is the great equalizer that makes it possible for all people to have opportunity to participate in the global research community. This talk focusses upon the need for education and research in developing countries where the opportunities are by isolation and lack of resources.
The African School for Electronic Structure Methods and Applications (ASESMA) has the goal to build up the scientific infrastructure that will give researchers in developing countries the opportunity to participate in the global scientific community. The long range goal is not limited to a narrow area of physics, but it started with an area of research that can be done at a world-class level with limited resources. Electronic Structure is based on fundamental principles of physics and is focused enough to allow collaborations and networking to build up a community within Africa. Yet it is widely used in physics, chemistry, materials science, and other fields. The key factor that has made it so useful is the advent of computational resources that are now available even in places where experimental facilities are prohibitively expensive.

ASESMA is a 10-year program endorsed by IUPAP and supported by various agencies, notably the ICTP. There are workshops each 2 years that have involved 171 participants from 18 countries, with ongoing efforts to support networking and collaboration between the schools. At present each school involves about 40 participants, half new to the field and half returning to continue interactions to build up his or her research. ASESMA has been critical for the success of many participants that are now advanced students, teachers, researchers and group leaders in Africa, and the leadership is developing to make ASESMA a truly African program.
The present series ends in 2020 and we are now creating a new vision for the future in computational materials science and other fields. There is the opportunity to have greater impact on many areas of education, science and technology by expanding and cooperating with other initiatives. The greatest need is for continuing support for work in Africa along with visits, collaborations, conferences, ... exactly what is needed for all people in research!

*Speaker

Nuclear Physics as Precision Science

Ulf-G Meißner *† [1]

[1] Universität Bonn and Forschungszentrum Jülich – Germany

Theoretical Nuclear Physics has entered a new era. Using the powerful machinery of chiral effective Lagrangians, the forces between two, three and four nucleons can now be calculated with unprecedented precision and with reliable uncertainties. Furthermore, Monte Carlo methods can be adopted to serve as a new and powerful approach to exactly solve nuclear structure and reactions. I discuss the foundations of these new methods and provide a variety of intriguing examples. Variations of the fundamental constants of Nature can also be investigated and the consequences for the element generation in the Big Bang and in stars are considered. This sheds new light on our anthropic view of the Universe.

*Speaker
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Multiscale Lattice Boltmann Simulations at the Physics-Biology Interface

Sauro Succi *† [1,2]

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Over the last near three decades, the Lattice Boltzmann (LB) method has gained a prominent role as an efficient computational scheme for the numerical simu- lation of complex states of flowing matter across a broad range of scales, from fully-developed turbulence in real-life geometries, to multiphase micro-flows, all the way down to nanofluidics and, lately, even quantum-relativistic subnuclear fluids. After a brief introduction to the main ideas behind the LB method, we shall illustrate a few selected multiscale applications to biological problems, such as biopolymer translocation across cell membranes, protein folding-aggregation and multiscale hemodynamics at cell resolution. Finally, we shall comment on the prospects of extreme LB simulations of biological organelles on future exascale computing platforms

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Astrophysics

Keynote: Gravitational waves: The new frontier of astrophysics

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LIGO's recent detections of gravitational-wave signals from several black-hole merger events not only confirm the century-old prediction of Einstein, but also herald the beginning of a new branch of astronomy. These observations provide us a first chance to test the predictions of Einstein's theory in the regime of extreme gravity, to study the physics of black holes and to probe the astrophysical formation channels of these binaries. Based on the observed rate of these events, we expect that a large number of black-hole mergers will be observed by LIGO and Virgo in the near future. This talk will summarize the current status of gravitational wave observations, what we learned from them, and prospects for the near future.

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Simulation of magnetorotational processes in core-collapsed supernovae

Sergey Moiseenko *† [1], Gena Bisnovatyi-Kogan [1]

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We represent results of numerical simulation of the magnetorotational(MR) mechanism of core-collapsed supernova explosion. Simulations were made using specially developed completely conservative Lagrangian operator-difference scheme on triangular grid of variable structure. We found the development of the Magneto-Differential-Rotational Instability(MDRI) during MR supernova explosion. The remapping of the grid is done in a special conservative way. The result of our simulations show that the explosion energy for MR supernova can reach up to the 2.5x10(51)ergs, what corresponds to the observations. The shape of the supernova explosion qalitatively depends on the initial configuration of the magnetic field. For the quarupole-like initial magnetic field the MR explosion develops mainly near the equatorial plane while for the dipole-like initial magnetic field we obtained mildly collimated axial jet.

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Modeling of Fragmentation and Density Stratification in the Process of Shock Interaction with Molecular Clouds on Grids with Very Large Resolution

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Numerical modeling was performed to study the processes of fragmentation, filament formation, and density stratification in molecular clouds (MC), in interaction with a shock wave (SW), or as a result of collision of MC with each other. One of the possible scenarios of such a process is the initiation of turbulent mixing in MCs shocked by a shock wave (SW) of supernova blast remnants (SNR). In this case turbulence of MC matter is accompanied by transient / reflected supersonic interaction of waves and leads to density fragmentation of MC's substance associated with the formation of filamentous structures in GMS. In this paper, we investigate the formation of instabilities of Richtmyer-Meshkov (RMI) and Kelvin-Helmholtz (KHI) that occurs in the boundary layers SW / ISM. The results of numerical simulation for two MCs on 3D large-scale computational grids up to 2048 $\times$ 1024 $\times$ 1024 are presented. The effect of the mass and shape of the cloud on the dissipation of the kinetic energy of the shock wave in the mixing zone, the formation of filaments and the stratification of the density are studied. The computations have shown that the formation of filaments and gas density stratification depend significantly on several factors. SWs interacting with MCs scatter their kinetic energy on ablating the cloud substance, forming regions of increased density and filaments.

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Nuclear, Particle and Fields Physics

Primary Vertex Reconstruction with the ATLAS experiment

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Efficient and precise reconstruction of the primary vertex in an LHC collision is essential in both reconstruction of the full kinematic properties of a hard-scatter event and in reconstruction of soft interactions as a measure of the amount of pile-up. The reconstruction of primary vertices in the busy, high pile-up environment of Run-2 of the LHC is a challenging task. New methods have been developed by the ATLAS experiment to reconstruct vertices in such environments. Advances in vertex seeding include methods taken from medical imaging, which allow for reconstruction of multiple vertices with small spatial separation. The adoption of this new seeding algorithm within the ATLAS adaptive vertex finding and fitting procedure will be discussed, and the first results of the new techniques from Run-2 data will be presented. Additionally data-driven methods to evaluate vertex resolution will be presented with special focus on correct methods to evaluate the effect of the beam spot constraint; results from these methods in Run-2 data will be presented.

*Speaker

Novel methods in track-based alignment to correct for time-dependent distortions of the ATLAS Inner Detector

Hide Oide [1], Shih-Chieh Hsu [2], Oscar Estrada * [3]

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ATLAS is a multipurpose experiment at the LHC proton-proton collider. Its physics goals require high resolution, unbiased measurement of all charged particle kinematic parameters. These critically depend on the layout and performance of the tracking system and the quality of its offline alignment. For the LHC Run II, the system has been upgraded with the installation of a new pixel layer, the Insertable B-layer (IBL). Offline track alignment of the ATLAS tracking system has to deal with about 700,000 degrees of freedom (DoF) defining its geometrical parameters, representing a considerable numerical challenge in terms of both CPU time and precision. An outline of the track based alignment approach and its implementation within the ATLAS software will be presented. Special attention will be paid to describe the techniques allowing to pinpoint and eliminate track parameters biases due to alignment. During Run-II, ATLAS Inner Detector Alignment framework has been adapted and upgraded to correct very short time scale movements of the sub-detectors. In particular, a mechanical distortion of the IBL staves up to 20um has been observed during data-taking. The techniques used to correct for this effect and to match the required Inner Detector performance will be presented.

*Speaker

The new ATLAS Fast Calorimeter Simulation

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Producing the very large samples of simulated events required by many physics and performance studies with the ATLAS detector using the full GEANT4 detector simulation is highly CPU intensive. Fast simulation tools are a useful way of reducing CPU requirements when detailed detector simulations are not needed. During the LHC Run-1, a fast calorimeter simulation (FastCaloSim) was successfully used in ATLAS. FastCaloSim provides a simulation of the particle energy response at the calorimeter read-out cell level, taking into account the detailed particle shower shapes and the correlations between the energy depositions in the various calorimeter layers. It is interfaced to the standard ATLAS digitization and reconstruction software, and it can be tuned to data more easily than GEANT4. Now an improved version of FastCaloSim is in development, incorporating the experience with the version used during Run-1. The new FastCaloSim makes use of statistical techniques such as principal component analysis, and a neural network parametrisation to optimise the amount of information stored in the ATLAS simulation infrastructure. A first prototype is available and is being tested and validated now. ATLAS plans to use this new FastCaloSim parameterization to simulate several billion events in the upcoming LHC runs. In this talk, we will describe this new FastCaloSim parametrisation.

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ATLAS Track reconstruction at the energy frontier

Shih-Chieh Hsu [1], Alex Kastanas * [2]

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ATLAS track reconstruction code is continuously evolving to match the demands from the increasing instantaneous luminosity of LHC, as well as the increased centre-of-mass energy. With the increase in energy, events with dense environments, e.g. the cores of jets or boosted tau leptons, become much more abundant. These environments are characterised by charged particle separations on the order of ATLAS inner detector sensor dimensions and are created by the decay of boosted objects. Significant upgrades were made to the track reconstruction code to cope with the expected conditions during LHC run 2. In particular, new algorithms targeting dense environments were developed. These changes lead to a substantial reduction of reconstruction time, while at the same time improving physics performance. The employed methods are presented and the prospects for future applications are discussed. In addition physics performance studies are shown, e.g. a measurement of the fraction of lost tracks in jets with high transverse momentum.

*Speaker

Keynote: Machine Learning from the proton structure to Higgs pair production at the LHC

Juan Rojo *† [1]

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TBA

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Statistical and systematic errors in the analysis of multiple datasets

Oleg Selyugin * [1], Jean-Rene Cudell *

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The different approaches to extraction of the parameters of interest for the combined datasets of independent experiments taking into account the systematic errors of each experimental set are analysed. It is shown that the frequency approach can give a larger χ^2 than the Bayesian approach, which takes into account the systematic errors with the prior in Gaussian form by the quadrature method but leads to a better estimation of the values of the model parameters. The analysis by maximum-likelihood method of different "gedanken" and real experimental data, obtained at the LHC, is presented. The results makes it possible to choose the best approach to obtaining the fitting model parameters, which are close to real values.

*Speaker

Transformed Lattice Rules for Feynman Loop Integrals

Elise De Doncker *† [1], Ahmed Almulihi [1], Fukuko Yuasa [2]

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[2] High Energy Accelerator Research Organization (KEK) – Japan

We focus on the application of rank-1 lattice rules with a transformation for the integration of functions which may have singularities on the boundaries of the integration domain. Using this technique we obtain results for Feynman loop diagrams including classes of 2-loop box diagrams and 3-loop self-energy diagrams having up to eight internal lines with masses. While lattice rules typically target problems with smooth integrand behavior, the integrals under consideration generally suffer from vanishing denominators on the boundaries of the (d-dimensional unit simplex) domain. We apply a tanh type transformaton in individual coordinate directions to map the integrand to zero at the boundaries of the transformed domain. The d-dimensional rule approximation with N points relies on a generator vector of length d with integer components, which is computed once and for all, and allows generating the N lattice points and corresponding integrand evaluations in a simple loop. We calculated the generator vector using the O(Nd log(N)) method by Nuyens and Cools, 2006) for rules of various numbers of points N and dimensions d. The generator vector is then incorporated in the integration program, which is implemented in CUDA for fast execution on GPUs. Results are provided efficiently and without special attention to specific problem characteristics.

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Atomic, Molecular and Optical Physics

Keynote: Towards controlled description of correlated fermions: diagrammatic Monte Carlo for the Hubbard model

Evgeni Kozik *† [1]

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Techniques of quantum field theory based on Feynman diagrams have been a powerful tool in many-body physics. Until recently, they have been employed either in low-order approximations or infinite sums of diagrams restricted to particular topologies. Development of the diagrammatic Monte Carlo (DiagMC) approach enabled access to high diagram orders and all topologies, potentially leading to unbiased results. On the other hand, it has revealed fundamental problems with Feynman diagrammatics, in particular suggesting a new scenario of breaking down of diagrammatic expansions. I will discuss how DiagMC can be used to address the Hubbard model on the square lattice in the region of moderate on-site repulsion U$<$ 4 (in the units of hopping t) and filling (number of fermions per lattice site) n$<$ 0.7 without uncontrolled approximations. In particular, I will present an accurate ground-state phase diagram in the (n,U) plane, describing competition between the p- and d-wave superfluid states. I will also focus on current limitations of the technique and show how some of them could be overcome by the example of the problem of pseudo-gap in the doped 2D Hubbard model.

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Numerical simulation of sympathetic cooling in radiofrequency ion traps for studies on antimatter

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The technique of sympathetic cooling by laser-cooled ions, allowing the preparation of cold and spatially localized ion ensembles, has found a wide range of applications; from quantum information technology to cold chemistry and high-precision spectroscopy [1]. In most experiments, the ions to be sympathetically cooled are produced in situ, e.g. by electron-impact ionization or photo-ionization from an atomic or molecular beam passing through the trap center. Our work focuses on a different and -up to now- much less studied experimental arrangement where ions are injected into the trap from an external ion source. In particular, this is required for antimatter ions, whose trapping and cooling is a crucial step of the GBAR project aiming to test the gravitational properties of antimatter [2,3]. Other applications include precision spectroscopy of highly charged ions [4] and studies on heavy molecular ions of biological interest created in electrospray ionization sources [5].

In view of the potentially large initial energy of the injected ions, the dynamics and efficiency of the sympathetic cooling process need to be understood in detail. To study this problem we have developed a molecular dynamics simulation code on GPU with a variable time step in order to represent correctly the Coulomb collisions experienced by fast ions [6]. Our results indicate that the process envisaged for the GBAR project (sympathetic cooling of positive antihydrogen ions by laser-cooled 9Be+) is very slow because of the unfavorable 9-to-1 mass ratio of the involved species. However, it may be greatly accelerated by introducing an additional ionic species of intermediate mass like HD+.

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C++QED: a framework for simulating open quantum dynamics – the first ten years

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C++QED is a versatile open-source C++/Python application-programming framework for simulating open quantum dynamics. It allows users to build arbitrarily complex interacting quantum systems from elementary free subsystems and interactions, and simulate their time evolution with a number of available time-evolution drivers. In my presentation, I will first sketch the outlines of C++QED, concentrating on two unique features:

(1) the fundamental design idea of the framework, which relies heavily on the multi-array concept and compile-time algorithms (C++ template metaprogramming)
(2) a modification of the Monte Carlo wave-function method to use adaptive time step.

Subsequently, I will present some important examples of usage that occured during the first decade of the history of the framework, some instructive limitations of the design, and the problems and challenges that C++QED has faced during this time and is facing nowadays.

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*Speaker

Quantum Many Body Physics

Importance of correlation effects for theoretical description of pressure induced electronic transitions: IMT, ETT, CLC.

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Structural and magnetic transitions upon compression are well known. However, the extreme pressure affects the electronic structure as well. Insulator-to-metal transitions (IMT) [1] and the topological changes of the Fermi surface for valence electrons, the so-called electronic topological transition (ETT) [2], represent well-known examples of the electronic transitions. They have attracted substantial interest due to controversial claims on their observations, e.g. in NiO, Zn and Os. We discuss the IMT in transition metal mono-oxides and in Fe2O3 [3], as well as ETT in hcp Fe [4] and Os [5,6]. We emphasize the importance of correlation effects in the theoretical treatment of the electronic transitions. Moreover, considering Os compressed to over 770 GPa, we discuss the anomaly observed experimentally in the behavior of the unit cells parameters ratio *c/a* at _˜440 GPa. We argue that the anomaly might be related to a new type of electronic transition, the core level crossing (CLC) transition, associated with interactions between the core electrons induced by pressure [5]. The generality of the CLC transitions is demonstrated in studies of other transition metals of the 6-th period [7].

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Keynote: Cluster multipole theory for anomalous Hall effect in antiferromagnets

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The anomalous Hall effect (AHE) occurs in solids with broken time-reversal symmetry. In early studies, the AHE was considered to arise in ferromagnets and scale with the magnetization of the system. On the other hand, it has been revealed in this decade that the AHE does not necessarily scale with the magnetization and it can arise even in antiferromagnets. Indeed, for some systems with non-coplanar spin configurations, the AHE occurs since the electrons feel a fictitious magnetic field characterized by the scalar spin chirality [1].

Recently, the AHE in systems with coplanar spin configurations is also attracting much interest [2,3,4,5]. In particular, the AHE in Mn3Sn[6] and Mn3Ge[7,8] is of great interest. There, the anomalous Hall conductivity is comparable to that of ferromagnetic metals, although neither the magnetization nor scalar spin chirality is finite. While the relation between the AHE and the topological properties of the electronic structure has been extensively studied[9], it is not fully understood whether there is a macroscopic quantity characterizing the AHE in coplanar antiferromagnets.

In this talk, we introduce a new order parameter, which we call cluster multipole (CMP) moment, and show that CMP quantifies the AHE in antiferromagnets with general spin configurations. In particular, we show that the antiferromagnetic states in Mn3Sn and Mn3Ge are characterized by a cluster octupole moment, and demonstrate the AHE in those antiferromagnets and that in elemental Fe can be discussed in the same scheme[10].

This work was done in collaboration with M.-T. Suzuki, T. Koretsune, and M. Ochi.

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*Speaker

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Assessing theoretical spectroscopy from novel first-principle approaches

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Understanding the spectroscopic properties of strongly correlated electron systems is one of the most important subjects in electronic structure theory. A proper theoretical description of the experimental observations is crucial for the understanding of many materials, but especially when effects of electronic correlations due to the Coulomb repulsion are important.
We will discuss the importance of the long ranged Coulomb interaction and nonlocal correlation effects within the combined many-body perturbation theory and dynamical mean-field theory (GW+DMFT) approach, which allows for assessing spectral properties beyond standard Density Functional Theory + DMFT methods.
We will present results obtained within GW+DMFT for transition metal compounds and discuss the effect of nonlocal correlations on the spectral function and Fermi surface.

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Recent Advances in Thermally-Assisted-Occupation Density Functional Theory (TAO-DFT)

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I will describe the formulation of our recently proposed thermally-assisted-occupation density functional theory (TAO-DFT) [1], the density functional approximations to TAO-DFT (TAO-DFAs) [2], and the hybrid TAO-DFT schemes (i.e., the inclusion of exact exchange in TAO-DFT) [3]. In contrast to Kohn-Sham density functional theory (KS-DFT), TAO-DFT is a density functional theory with fractional orbital occupations given by the Fermi-Dirac distribution (controlled by a fictitious temperature), for the study of large ground-state systems with strong static correlation effects [4,5,6,7]. However, existing exchange-correlation energy functionals in KS-DFT may also be adopted in TAO-DFT. Besides, TAO-DFT has similar computational cost as KS-DFT for single-point energy and analytical nuclear gradient calculations, and reduces to KS-DFT in the absence of strong static correlation effects. Relative to our previous TAO-DFAs, the hybrid TAO-DFT schemes are shown to be superior in performance for a broad range of applications, such as thermochemistry, kinetics, and reaction energies.

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Doping dependence of charge order in electron-doped cuprate superconductors

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The recently discovered charge order is a generic electronic property of both the hole- and electron-doped cuprate superconductors [1,2], where a central issues is what mechanism causes the charge-order formation. Within the framework of the t-J model in the fermion-spin representation [3,4], the doping dependence of charge order in the electron-doped cuprate superconductors is studied by taking into account the electron self-energy effect (then the strong electron correlation effect) [5]. It is shown that as in the hole-doped cuprate superconductors [6], the charge-order state in the electron-doped cuprate superconductors is also driven by the Fermi-arc instability, with a characteristic wave vector corresponding to the hot spots of the Fermi arcs, therefore there is a common physical origin for the charge-order correlation in both the hole- and electron-doped cuprate superconductors. However, in a striking contrast to the hole-doped case [6], the magnitude of the charge-order wave vector in the electron-doped side increases almost linearity with the increase of doping. The theory also indicates that the Fermi-arc instability generated charge-order state in cuprate superconductors is intimately related to the strong electron correlation induced electron self-energy.

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*Speaker

Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of multireference perturbation theory

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A hybrid stochastic-deterministic approach for computing the second-order perturbative contribution E (2) within multireference perturbation theory (MRPT) is presented. The idea at the heart of our hybrid scheme - based on a reformulation of E (2) as a sum of elementary contributions associated with each determinant of the MR wave function - is to split E (2) into a stochastic and a deterministic part. During the simulation, the stochastic part is gradually reduced by dynamically increasing the deterministic part until one reaches the desired accuracy. In sharp contrast with a purely stochastic Monte Carlo scheme where the error decreases indefinitely as the inverse square root of the computational time, the statistical error in our hybrid algorithm converges with a typical exponential-like behavior. If desired, the calculation can be carried on until the stochastic part entirely vanishes. In that case, the exact (deterministic) result is obtained with no error bar and no noticeable computational overhead compared to the fully-deterministic calculation. The method is illustrated on the F2 and Cr2 molecules. Even for the largest case corresponding to the Cr2 molecule treated with the cc-pVQZ basis set, very accurate results are obtained for E (2) for an active space of (28e,198o) and a MR wave function including up to 2.8 $\times$ 10^7 determinants.

*Speaker

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Proposal of a new fully uncontracted multi-reference perturbation theory

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Strongly correlated systems are of prime importance in chemistry and material science because of their exotic electronic structure. From a theoretical point of view, such systems are characterized by the existence of several nearly degenerated electronic configurations which are needed for a qualitative description of the system, defining the zeroth-order wave function. However, the quantitative description of many important quantities as excitation energies and binding energies requires a more careful description of the electronic correlation arising at short inter-electronic distances, generally called dynamical correlation. More precisely, one needs to describe correctly each of the electronic configurations of the zeroth-order wave function, which is the realm of the so-called multi-reference (MR) techniques.

In this presentation, I will present a new MR perturbation theory at second order (MRPT2) which accounts for such effects in a quite cheap and efficient way. A crutial aspect of the present formalism is that it respects the size consistency property, which is fundamental for the computation of energy differences. Also, the formulation of the perturbation theory as an effective hamiltonian allows to take into account the influence of the dynamic correlation on the structure of the zeroth-order wave function, which is crutial when the coupling between long and short range correlation effects is large.

After presenting briefly the key concepts of such a new formalism, I will show numerical examples on strongly correlated model systems, such as diatomic molecules and transition metal complexes. Also, the effective hamiltonian formulation allows for a clear understanding of the physical effect of the dynamic correlation effects, whic I will illustrate numerically.

*Speaker

Off-Diagonal Expansion Quantum Monte Carlo

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I will present a novel Monte Carlo algorithm designed to simulate quantum as well as classical systems at equilibrium, bridging the algorithmic gap between quantum and classical thermal simulation algorithms. The method is based on a new decomposition of the quantum partition function that can be viewed as a series expansion about its classical part. I will argue that the algorithm is optimally suited to tackle quantum many-body systems that exhibit a range of behaviors from 'fully-quantum' to 'fully-classical'. I will demonstrate some of the advantages of the technique by comparing it against existing schemes and illustrate how this method allows for the unification of quantum and classical thermal parallel tempering techniques into a single algorithm.

*Speaker

Coupled Electron-Ion Monte Carlo study of hydrogen under extreme conditions

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The phase diagram of high pressure hydrogen is of great interest for fundamental research, planetary physics, and energy applications[1]. Laboratory experiments to reach the appropriate thermodynamics conditions are difficult and extremely expensive, therefore ab-initio theory has played a crucial role in developing the field. The accuracy of Density Functional based calculations is however limited and often non-predictive. We have developed a quantitative methodology based on Quantum Monte Carlo to study hydrogen in extreme conditions: the Coupled Electron-Ion Monte Carlo (CEIMC). We will report results for a number of studies we have recently performed.
The first application of CEIMC is in computing the principal Hugoniot of deuterium[2]. We find that the maximum compression along the Hugoniot is _˜5% higher than with DFT and _˜15% higher than most accurate experimental data[3].

A second application is to tracing the liquid-liquid transition line. A first-order phase transition in the fluid phase between a molecular insulating fluid and a monoatomic metallic fluid has been predicted[4-6]. The existence and precise location of the transition line is relevant for planetary models. Recent experiments reported contrasting results about the location of the transition[7-9]. Theoretical results based on density functional theory are also very scattered[8]. We report highly accurate coupled electron-ion Monte Carlo calculations of this transition finding results that lie between the two experimental predictions, close to that measured in diamond anvil cell experiments but at 25-30 GPa higher pressure. The transition along an isotherm is signaled by a discontinuity in the specific volume, a sudden dissociation of the molecules, a jump in electrical conductivity and loss of electron localization[10]. We discuss the difference observed with respect to the predictions of a different Quantum Monte Carlo method [11].

Finally a third application of CEIMC is to study the stability of the various crystalline molecular phases of hydrogen. We have performed calculations along the T=200K isotherm in the phase III and along the T=414K isotherm in the phase IV. We report a preliminary comparison between CEIMC results and DFT based results and discuss the electronic character of the various phases[12].

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Quantum spin phases emerged from the interplay between strong correlation and spin-orbital coupling

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The search for the exotic quantum phases constitutes one of the most important and hot issues in modern condensed matter physics. Here, I plan to present our recent theoretical investigations on the quantum phases and quantum phase transitions in the Hubbard model on the triangular lattice with spin-dependent Kitaev-like hopping. Using the variational cluster approach, we map out its phase diagram, which contains a non-coplanar chiral magnetic order, an extended nonmagnetic insulating phase (NMI), and an interacting Chern insulator (CI). The transition from CI to NMI is characterized by the change of the charge gap from an indirect band gap to a direct Mott gap. The nonmagnetic insulator has been further classified into a gapless spin liquid with a spinon Fermi surface and a fractionalized Chern insulator with nontrivial spinon topology. In addition, we derive a minimal effective spin model from the five-orbital Hubbard model with spin-orbital coupling using the energy bands obtained from the first-principle calculations for α-$RuCl_3$. The minimal model contains the ferromagnetic Kitaev term and the antiferromagnetic off-diagonal exchange term. Based on this model, we investigate the spin-wave excitation using the SU(N) linear spin wave theory and find it is consistent with the recent neutron scattering on α-$RuCl_3$. It demonstrates that the Kitaev interaction, the concept central to the Kitaev quantum spin liquid, is realized in α-$RuCl_3$.

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*Speaker

Towards exascale simulations of quantum superfluids far from equilibrium

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Superfluidity is a generic feature of various quantum systems at low temperatures. It has been experimentally confirmed in many condensed matter systems, in ^{3}He and ^{4}He liquids, in nuclear systems including nuclei and neutron stars, in both fermionic and bosonic cold atoms in traps, and it is also predicted to show up in dense quark matter. The time dependent density functional theory (TDDFT) is, to date, the only microscopic method which allow to investigate fermionic superfluidity far from equilibrium. The local version of TDDFT is particularly well suited for leadership class computers of hybrid (CPU+GPU) architecture. Using the most powerful supercomputers we are currently able to study a real-time 3D dynamics without any symmetry restrictions evolving up to hundred of thousands of superfluid fermions. It represents a true qualitative leap in quantum simulations of nonequilibrium systems, allowing to make quantitative predictions and to reach limits inaccessible in laboratories. During the talk I will review several applications and results concerning nuclear induced fission and collisions, dynamics of nuclear matter in neutron stars, dynamics of topological excitations in ultracold atomic clouds and prospects to produce a quantum turbulent flow.

*Speaker

Simulations of electron energy loss spectra with turboEELS

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Plasmonics is a rapidly developing branch of nanophysics, as it proposes a variety of tools that can be used both in research and industry (i.e. plasmonic waveguides, near field microscopes, surface plasmon resonance sensors, etc), so plasmons and their properties have been extensively studied during last decades both experimentally and theoretically. From the theoretical point of view it is necessary to have a tool that allows to characterise and study plasmons in an accurate and efficient way. In this project we use the Liouville-Lanczos algorithm implemented in the turboEELS code [1,2] of Quantum ESPRESSO. We compute the electronic susceptibility in time-dependent density functional perturbation theory (TDDFPT) and simulate electron energy loss spectra (EELS) in order to study surface plasmons in noble metals (Au, Ag, Cu) with the main focus on gold surfaces. In previous studies of surface plasmons in Au, spin-orbit coupling was not taken into the account [3], while it is known that this effect influences band structure significantly. In our project we would like to emphasise the importance of spin-orbit coupling and to perform full relativistic study of EEL spectra for Au surfaces. In particular, we have already shown that there is non-negligible difference between EELS of bulk Au with and without spin-orbit coupling. In order to perform the efficient study we are implementing the spin-orbit coupling interaction with ultrasoft pseudopotentials in the turboEELS code. Performance of the turboEELS code will also be presented on bismuth [4] and on silicon.

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*Speaker

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Spin-Charge Coupling in Unconventional Superconductors: Insights from Diffusion Monte Carlo

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We show that diffusion Monte Carlo provides a faithful description of magnetism in transition metal pnictide compounds, some of which are high temperature superconductors. Our results highlight the importance of spin-charge coupling as a key normal state ingredient for high temperature superconductivity in both iron-based and copper-based superconductors. Based on an analysis of charge response to magnetic order, within this accurate diffusion Monte Carlo framework, we introduce a spin-charge coupling descriptor that separates superconducting materials from non-superconducting ones. Such a calculable descriptor could pave the way for theory-guided search for new unconventional superconductors and provide interesting guidance for modifying known materials to perhaps find superconductivity.

*Speaker

Ab initio approach to strong correlations in lanthanide compounds: from localized magnets to heavy-fermions.

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We review some recent applications of the density-functional+dinamical-mean-field-theory (DFT+DMFT) *ab initio* framework to rare-earth compounds.
First, a DFT+DMFT framework for evaluating the crystal and exchange-field parameters in lanthanides is presented and its applications to hard-magnetic rare-earth intermetallics are discussed. In these compounds the 4*f* shells remain strongly localized and can be treated within a quasi-atomic (Hubbard-I) approximation. The coupling of 4*f*s to the transition-metal sublattice through crystal-field (CF) and exchange fields as well as due to hybridization effects determines the magnetic anisotropy and, hence, the magnetic hardness of those compounds. The DFT+DMFT calculations of the CF splitting in new rare-earth-based hard magnets of the *R*Fe12*X* family (*R*=Nd,Sm) predict a change of sign of the key CF parameter determining the anisotropy upon the substitution of the interstitial *X*=N with Li. We thus find a large out-of-plain anisotropy for NdFe12N but also for the hypothetical SmFe12Li hard magnet. The effect of interstitials N and Li on the CF splitting is clarified by an analysis of the 4*f* Wannier orbitals and their leakage to the interstitial sites.

A different application of DFT+DMFT to lanthanides concerns Ce-based heavy-fermion (HF) compounds. In this case a change in external parameters (pressure, temperature) induces crossovers between the local-moment (LM) and HF behavior as well as between different HF regimes. We apply DFT+DMFT to study the evolution of the spectral function, orbital occupancy and Fermi surface (FS) at those crossovers. The local many-body problem for Ce 4*f* shell was solved using continuous-time Monte Carlo method. We find a drastic difference between CeNiAsO and CeNiPO upon lowering the temperature: while the former keeps the "small" FS of the LM regime, a significant FS reconstruction is predicted for the later upon the onset of HF behavior [1]. In CeCu2Si2 and CeAu2Si2 [2,3] we find a pressure-induced FS reconstruction accompanied by a change of the orbital state of Ce 4*f* electron. We assign this reconstruction to an orbital transition between two distinct HF regimes.

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Dynamics of nuclear fission within the time-dependent generator coordinate method

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The dynamics of nuclear fission represents a time-dependent many-body problem which involves more than 200 nucleons and still challenges nuclear theory. During this process, an excited atomic nucleus deforms up to a point where it suddenly breaks into two main fragments. One of the current stack in this topic consists in predicting the distribution of mass and charge of the fragments from the collective motion of the system toward its splitting. In this context, a promising theoretical framework is the time dependent generator coordinate method (TDGCM) applied under the Gaussian overlap approximation (GOA). However, the computational cost of this method was up to now a hurdle to perform accurate realistic calculations with two and more collective degrees of freedom. To overcome this limitation, we develop the code FELIX aiming to solve the time dependent Schr$^{'}$odinger equation risen by this formalism, for an arbitrary number of collective variables.
In this talk, we will present the numerical methods adopted as well as the status of the latest version of FELIX. We will then discuss the success and limits of the TDGCM+GOA approach with recent results on the low energy fission.

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Carbon nanotubes as excitonic insulators

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Fifty years ago Walter Kohn speculated [1] that a zero-gap semiconductor might be unstable against the spontaneous generation of excitons-electron-hole pairs bound together by Coulomb attraction. The reconstructed ground state would then open a gap breaking the symmetry of the underlying lattice, a genuine consequence of electronic correlations. Here we show [2] that this 'excitonic insulator' is realized in zero-gap armchair carbon nanotubes by performing first-principles calculations through many-body perturbation theory as well as quantum Monte Carlo. The excitonic order modulates the charge between the two carbon sublattices opening an experimentally observable gap, which scales as the inverse of the tube radius and weakly depends on the axial magnetic field. Our findings confute the Luttinger liquid paradigm for nanotubes and provide tests to experimentally discriminate between excitonic and Mott insulator.

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*Speaker

Connected Determinant Diagrammatic Monte Carlo: polynomial-time complexity thanks to the fermionic sign

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In this talk, I will present a simple, versatile, and very efficient technique to compute fermionic diagrammatic expansions at high order [1]. Considering the sum of all connected Feynman diagrams at once allows one to take the thermodynamic limit analytically, and to take into account the large cancellations between different diagram topologies automatically, which greatly reduces the computational effort.
In addition, we will see that for convergent (or resummable) fermionic diagrammatic series computed with this algorithm, the computational time increases only polynomially with the inverse error on thermodynamic-limit quantities [2].

[1] arXiv:1612.05184
[2] arXiv:1703.10141

*Speaker

Nature of Quasi-Particle Excitations in the Spin-1/2 Square-Lattice Heisenberg Antiferromagnet

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We study the spin excitation spectrum (dynamic structure factor) of the spin-$1/2$ square-lattice Heisenberg antiferromagnet. Using an improved method for analytic continuation of the corresponding imaginary-time correlation functions computed with quantum Monte Carlo simulations, we can treat the sharp (δ-function) contribution expected from spin-wave (magnon) excitations in addition to a continuum above the magnon energy. The results are in excellent agreement with recent neutron scattering experiments on the almost ideal Heisenberg system $Cu(DCOO)_{24}D_2O$, where it was argued that no magnon δ-function exists at wavenumber $q = (\pi, 0)$ and this was interpreted as spinons, i.e., fractional excitations carrying half of the spin of a magnon. Our results instead show a significant reduction, not complete suppression, of the magnon weight and a large continuum. The excitation continuum has traditionally been ascribed to multi-magnon processes, but we show here that an alternative interpretation is that it originates from virtual spinons. We introduce a simple effective model of the excitations in which a magnon can decay into two spinons that do not separate but fluctuate in and out of the magnon space. The model can reproduce the reduction of the magnon weight and lowered excitation energy at $q = (\pi, 0)$ as well as the opposite trend (also seen experimentally) at $q = (\pi/2, \pi/2)$. Based on these results, we reinterpret the picture of deconfined spinons at $q = (\pi, 0)$ in the experiments as nearly deconfined spinons. This interpretation is further supported by calculations for a model where the Heisenberg exchange J is supplemented by a multi-spin interaction Q (the J-Q model) that can bring the system to a deconfined quantum critical point. In the analytically continued spectrums we observe that the magnon δ-function vanishes at $q = (\pi, 0)$, but not at $q = (\pi/2, \pi/2)$, even with a weak Q-coupling, much before the deconfinement transition (which is the point at which the low-energy spinons deconfine). Our conclusion is that spinons play an important role in Heisenberg systems such as $Cu(DCOO)_{24}D_2O$ even though they are not fully deconfined, and also suggest that full deconfinement close to $(\pi, 0)$ may be possible in other materials where higher-order interaction effects, such as longer-range couplings or cyclic exchange.

*Speaker

Controlled summation of diagrammatic series for the unitary Fermi gas: bold diagrammatic Monte Carlo, large-order asymptotics and conformal-Borel transformation

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We consider the unitary Fermi gas (spin $1/2$ fermions with contact interactions in three-dimensional continuous space, a model which accurately describes cold atomic gases at a Feshbach resonance and is also relevant to neutron matter) in the normal phase. Thanks to a diagrammatic Monte Carlo algorithm, we accurately sample all skeleton diagrams (built on dressed single-particle and pair propagators) up to order 8 [1]. The diagrammatic series is divergent and there is no small parameter so that a resummation method is needed. Previously we used Abelian resummation methods, which are applicable under the assumption that the diagrammatic series has a non-zero radius of convergence; this led to good agreement with cold atom experimental data for the equation of state [2] and Tan's contact coefficient [3]. Here we report the large-order asymptotics of the diagrammatic series, based on a functional integral representation of the skeleton series [4] and the saddle-point method. We find that the radius of convergence is actually zero, and our preliminary numerical results and analytical arguments suggest that the series is resummable by an generalised conformal-Borel transformation that incorporates the large-order asymptotics.

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*Speaker

Keynote: Gapless Spin-Liquid Ground State in the S=1/2 Kagome Antiferromagnet

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The defining problem in frustrated quantum magnetism, the ground state of the nearest-neighbor spin 1/2 antiferromagnetic Heisenberg model on the kagome lattice, has defied all theoretical and numerical methods employed to date. We apply the formalism of tensor-network states, specifically the method of projected entangled simplex states, which combines infinite system size with a correct accounting for multipartite entanglement. By studying the ground-state energy, the finite magnetic order appearing at finite tensor bond dimensions, and the effects of a next-nearest-neighbor coupling, we demonstrate that the ground state is a gapless spin liquid. We discuss the comparison with other numerical studies and the physical interpretation of this result.
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Dephasing and disorder effects in the topological systems

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The influence of dephasing and disorder effects in the topological systems, such as the quantum spin Hall effect (QSHE) system, the surface states of 3D topological insulators, and the Weyl semimetals (WSMs) is studied. For the 2D QSHE system, we find that the quantum conductance plateaus are robust against the normal dephasing but fragile with the spin dephasing, and thus these quantum plateaus only survive in mesoscopic samples. For the surface states of 3D topological insulators, we show that the combination of dephasing and impurity scattering can cause backscattering in the helical states. In WSMs, we predict the Goos-H$^{'}$anchen and the Imbert-Fedorov shifts exist for the reflection at the interface of two WSMs. We find that the IF shift originates from the topological effect of the system, and can be utilized to characterize the Weyl semimetals, to design valleytronic devices, and to measure the Berry curvature of the system. We also study the impurity scattering and disorder effects in the WSMs. We show that the topological IF shift also influences the single impurity scattering cross-section and gives rise to exotic transport properties of WSMs. Furthermore, we study the disorder induced localization in WSMs, and find three exotic quantum phase transitions.

*Speaker

Short-time quantum critical dynamics for Ising model in a transverse eld

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We study the short time behavior of the transverse eld Ising model(TFIM) with projector quantum Monte Carlo(QMC) in both one and two dimension. In the early stage of evolution, we extract the critical point and static exponent beta/nu and another important critical exponent theta called initial slip exponent through nite size scaling analysis. We obtain high-precision estimates of the quantum critical point (h/J)c = 1:00003(8) and (h/J)c = 3:04451(7) for the one and two dimensional TFIM, respectively. The critical exponents are theta = 0:3737(5), beta/nu = 0:1250(3) for the one dimensional case and theta = 0:192(6), beta/nu = 0:5229(7) for the two dimensional case.

*Speaker

Diagrammatic extensions of DMFT: Nonlocal interactions and nonlocal correlations

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The Coulomb interaction between electrons leads to correlation and to deviations from the single-particle picture. The combination of Dynamical Mean-Field Theory with band-structure methods has allowed the study of the local interaction and correlation effects. Over the last decade, several approaches have been developed with the goal of also incorporating *nonlocal* effects on top of Dynamical Mean-Field theory. These nonlocal effects are especially important in two-dimensional systems, where screening is strongly reduced. In this talk, I will discuss recent results obtained using the "dual boson" extension of Dynamical Mean-Field Theory, showing the effect of nonlocal interactions on the collective excitation spectra and on phase transitions of strongly correlated electron systems.

*Speaker

Classical Statistical Mechanics

Random Field Ising Model with Conserved Kinetics: Super-Universality Violation, Logarithmic Growth Law and the Generalized Tomita Sum Rule

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We perform comprehensive Monte Carlo (MC) simulations to study ordering dynamics in the random field Ising model with conserved order parameter (C-RFIM) in $d = 2, 3$. The observations from this study are: (a) For a fixed value of the disorder Δ, the correlation function $C(r, t; \Delta)$ exhibits dynamical scaling. (b) The scaling function is not robust with respect to Δ, i.e., super-universality (SU) is violated by $C(r, t; \Delta)$. (c) At early times, the domains follow algebraic growth with a disorder-dependent exponent: $L(t, \Delta) \sim t^{1/\tilde{z}(\Delta)}$. At late times, there is a cross-over to logarithmic growth: $L(t, \Delta) \sim (\ln t)^{1/\varphi}$, where φ is a disorder-independent exponent. (d) The small-r behavior of the correlation function exhibits a *cusp singularity*: $1 - C(r) \sim r^{\alpha(\Delta)}$, where α is the *cusp* exponent signifying rough fractal interfaces. (e) The corresponding structure factor exhibits a *non-Porod* tail: $S(k, t; \Delta) \sim k^{-(d+\alpha)}$, and obeys a *generalized Tomita sum rule* $\int_0^\infty \mathrm{d}p\, p^{1-\alpha} \left[p^{d+\alpha} f(p) - \mathcal{C}\right] = 0$, where $f(p)$ is the appropriate scaling function, and $\mathcal{C}$ is a constant.

*Speaker

GPU accelerated population annealing algorithm and its application to first- and second-order phase transitions

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Population annealing is a promising recent approach for Monte Carlo simulations in statistical physics, in particular for the simulation of systems with complex free-energy landscapes. It is a hybrid method, combining importance sampling through Markov chains with elements of sequential Monte Carlo in the form of population control. While it appears to provide algorithmic capabilities for the simulation of such systems that are roughly comparable to those of more established approaches such as parallel tempering, it is intrinsically much more suitable for massively parallel computing.
Here, we tap into this structural advantage and present a highly optimized implementation of the population annealing algorithm on GPUs and obtain speed-ups of several orders of magnitude as compared to a serial implementation on CPUs. Our code includes implementations of some advanced algorithmic features that have only recently been suggested, namely the automatic adaptation of temperature steps and a multi-histogram analysis of the data at different temperatures.

Systems with first-order phase transitions are among the problems in computational physics that are difficult to tackle with standard methods such as local-update simulations in the canonical ensemble, for example with the Metropolis algorithm. It is hence interesting to see whether such transitions can be more easily studied using population annealing. We report our preliminary observations from population annealing runs for the two-dimensional Potts model with $q > 4$, where it undergoes a first-order transition.

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*Speaker

Phase transitions in evolutionary space games

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We study the dynamics of a space evolutionary game based on the prisoners' dilemma. The game features a series of sharp transitions between several regimes, characterized by abrupt changes in the densities of the components and non-trivial geometric rearrangements of the game field. We investigate critical properties of the resulting phase transitions and discuss the geometric properties of the emergent interfaces between components.

*Speaker

Deep Learning for Fatigue Estimation on the Basis of Multimodal Human-Machine Interactions

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Physiological signals can be categorized into cerebral (electroencephalography, functional magnetic resonance imaging, etc.) and peripheral (heart rate, biological activity, temperature, etc.) ones. Due to development of wearable electronics and Internet of Things, these complex physicochemical signals can be recorded and transmitted from various limbs, and then they can be statistically analyzed as an integral set of multimodal human-machine interactions. Here the new method is proposed to monitor the level of currently accumulated fatigue and estimate it by the several statistical and machine learning methods. The data from brain-computing interface (electroencephalography) and peripheral sensors (accelerometer, GPS, gyroscope, magnetometer) were collected, integrated, and analyzed by several statistical and machine learning methods (moment analysis, cluster analysis, principal component analysis, etc.). The hypothesis 1 (physical activity can be classified) and hypothesis 2 (fatigue level can be estimated quantitatively and distinctive patterns can be recognized) were proposed and proved. Several "fatigue metrics" were proposed and verified on several persons of various age, gender, fitness level, etc. The method can be used in practice for ordinary people in everyday situations (to estimate their fatigue, give tips about it and advice on context-related information).

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Large deviations for equilibrium and non–equilibrium processes

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Large deviations and rare events play an ever increasing role in science, economy and society. Large deviations play a crucial role for example for the estimation of impacts of storms, the calculation of probabilities of stock-market crashes or the sampling of transition paths for conformation change of proteins. More fundamentally, when studying any random process, only the full probability distribution, including the large-deviation tails, gives a complete information about the underlying system. The basic principal to study large deviations using numerical simulations is simple: make unlikely events more probable and correct in the end for the bias [1]. Here, we present a very general black-box method [2], based on sampling vectors of random numbers within an artificial finite-temperature (Boltzmann). This allows to access rare events and large deviation for almost arbitrary equilibrium and non-equilibrium processes. In this way, we obtain probabilities as small as 10–500 and smaller, hence rare events and large-deviation properties can be easily obtained.

The method can be applied to equilibrium/static sampling problems, e.g., the distribution of the number and size of connected components of random graphs [3,4]. Here, applications from different fields are presented: • Distribution of work performed for a critical ($T = 2.269$) two-dimensional Ising system of size $L \times L = 128 \times 128$ upon rapidly changing the external magnetic field [2] (also applying theorems of Jarzynski and Crooks to obtain the free energy difference of such a large system) • Distribution of perimeters and area of convex hulls of two- and higher dimensional single and multiple random walks [5,6] • Distribution of the flow for the Nagel-Schreckenberg traffic model. Other recent applications where probability distributions over a large range of the support and down to extremely small probabilities were obtained using such approaches include biological sequence alignments [7,8,9], chemical similarity assessment [10], RNA secondary structures [11], minimum-energy paths on hierarchical lattices [12], spin glass ground states [13], structure of energy grids [14,15], and calculation of partition functions of Potts models [16].

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Computations of self-assembly of rod-like particles on a plane

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In recent decades, much attention has been paid to the study of phase behavior and self-assembly in dense two-dimensional (2D) systems of hard rods. A linear k-mer (particle occupying k adjacent adsorption sites) represents the simplest model of a rod with an aspect ratio of k. Computer simulations have been extensively applied to investigate percolation and jamming phenomena for the random sequential absorption (RSA) of k-mers, and various anomalies in the properties of the systems' dependence on the length of the k-mers have been reported [1–6].
In this work the diffusion-driven self-assembly of the k-mers was studied by means of kinetic Monte Carlo simulation. The initial jamming state was produced using RSA algorithm with isotropic orientations of the k-mers, the k-mers were allowed to diffuse. In such dense systems, only the translational diffusion of particles is possible, whereas rotational diffusion is completely inhibited. The length of the k-mers (aspect ratio) was varied from 2 to 12. The size of lattice, L, was varied from 128 to 2048, and periodic boundary conditions were applied to the lattice along both the x and y directions. For characterization of diffusion-driven processes the number of intraspecific / interspecific contacts between the different sorts of k-mers and the electrical conductivity of the system were evaluated. The systems under consideration exhibited the rich non-equilibrium patterning. Quite different self-organization behavior was observed for short and long k-mers. The most striking was the formation of diagonal stripe domains for aspect ratios above a specific critical value, $k \geq 6$. The three main stages of diffusion-driven spatial segregation (self-assembly) were identified: the initial stage, reflecting destruction of the jamming state, the intermediate stage, reflecting continuous cluster coarsening and labyrinth pattern formation and the final stage, reflecting the formation of diagonal stripe domains. For shorter k-mers ($k \leq 5$), the diagonal patterns did not occur. The observed effects surely reflect the competition between different factors related to the discrete nature of the rods, the limited numbers of their possible orientations and the finite sample size. The effects of k-mer length, anisotropy of deposition, presence of defects, vertical drying and diffusion-driven self-organizations on behaviour of electrical conductivity have also been investigated.

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Keynote: Scalable and efficient first-principles based Monte Carlo simulations on high performance computers

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Classical Monte Carlo methods are one of the most robust and widely-used computational techniques to study statistical mechanics of physical systems. Modern supercomputers make it possible to combine Monte Carlo with first-principles methods, such as the Density Functional Theory (DFT), for the evaluation of energy and thermodynamic properties. Such approach is proven to be effective in carrying out highly accurate simulations that are comparable with experimental observations. A previous, successful example is WL-LSMS [1], which combines the Wang-Landau (WL) Monte Carlo algorithm [2] with a DFT method, Locally Self-consistent Multiple Scattering (LSMS) [3], for the study of phase transitions of magnetic materials and alloys. While LSMS scales across multiple compute-nodes linearly with the system size, Wang-Landau sampling is a serial algorithm by construction like most Monte Carlo algorithms, which imposes a serious bottleneck for making good use of the massive computing power of future high performance computers. We tackle this problem by introducing new Monte Carlo algorithms to improve strong and weak scaling. Firstly, the parallel framework for Wang-Landau sampling, namely Replica-Exchange Wang-Landau sampling [4], is employed to invoke an additional level of parallelism that utilizes multiple Monte Carlo walkers. Secondly, a histogram-free multicanonical method [5] is proposed, which can reduce the number of Monte Carlo steps required to converge the simulations by approximately one order of magnitude. We will demonstrate how these novel algorithms are able to decrease the simulation time for obtaining the density of states for a simulated system dramatically, thus accelerating scientific discovery.

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Vapor nucleation under extreme confinement.

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Vapor nucleation under extreme confinement.
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Textured surfaces, characterized by hierarchical micro and nano cavities, enhance their *chemical* hydrophobicity and have many technological emerged and submerged applications, such as drag reduction, anti-fouling, self-cleaning, etc. On textured surfaces liquids can stay suspended over the gas layer entrapped in the surface cavities (Cassie-Baxter state), and their intriguing properties are maintained as long as the liquid does not invade surface corrugations. Thus, ideal materials must be able to prevent the wetting transition or, in case it happens triggered from some external perturbation, the system can readily *self-recover* the suspended state.

The self-recovery process consists in the nucleation of a gas or vapor bubble in the micro and nanoscopic surface cavities. Investigating gas/vapor nucleation in confined liquids is a scientific challenge for many reasons. First of all, nucleation is a rare event, i.e. an event tacking place only once in a while with a characteristic time that might be inaccessible to standard simulations or even experiments [1]. This is because the system is characterized by metastabilities, i.e. the presence of an absolute and local minima of the free energy separated by a large barrier, much higher than the thermal energy available to the system, kBT. In the case of confined liquids, the stable and metastable states correspond to the liquid filling or leaving empty the confining cavities. Gas/vapor nucleation takes place when the metastable state with liquid in the cavities overcomes the nucleation barrier forming a critical bubble, which, then, expands up to completely emptying the cavities.

Understanding how nucleation barrier is affected by the morphology, size and chemistry of the confining cavities is important for technological applications (those mentioned above and many more) and intriguing from a fundamental point of view. In fact, nucleation in confined systems cannot be investigated taking as reference well established theories, such as the classical nucleation theory - CNT, because confinement imposes constraints on the shape of bubbles, which are neither of spheres nor spherical caps as predicted by bulk and heterogeneous CNT. At the same time, doubts have been casted on the model necessary to represent the multiphase system at the nanoscopic level of confinement, for example whether the sharp interface model, the simplest and reference model in nucleation, is adequate down to the nanoscopic scale. Thus, many fundamental aspects remain to be addressed and new theories need to be developed.

*Speaker

We investigated confined nucleation in a set of systems characterized by different geometries, size and chemistry using special simulation techniques (restrained molecular dynamics [1], string method [2], forward flux) in combination with continuum [3] and atomistic models of the liquid. In my contribution I will discuss the mechanism of nucleation under extreme confinement, showing the complex path of formation and growth of bubbles, with their change of morphology along the process, the associated energetics and its dependence on the physical and chemical characteristics of cavities. Surprising is the fact that the very simple sharp interface model is able to capture the main qualitative and semi-quantitative characteristics of these *non-classical* mechanisms and energetics of confined nucleation, provided that one uses it in combination with simulation techniques able to identify the realistic nucleation path. I will also show how from our simulations is possible to derive design principles for self-recovery superhydrophobic surfaces with texturations ranging from nano to macroscopic sizes.

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Melting transition of skyrmion lattice in a two-dimensional chiral magnet

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Skyrmions are topologically stable particles which appear in magnetic systems, as non-trivial spin textures typically composed of tens of spins. The skyrmion in magnetic systems is stabilized by various mechanisms such as the antisymmetric Dzyaloshinskii–Moriya (DM) interaction and frustrated exchange interactions. Recently many experimental studies observe the magnetic skyrmions in chiral magnets with the DM interaction like MnSi. Magnetic skyrmions in three-dimensional chiral magnets are thermodynamically stable only as a skyrmion lattice. In contrast to the three-dimensional case, isolated skyrmions are also stable at finite temperature in two dimensionsand a melting transition from a lattice phase to a gas phase characteristic of two- dimensional case occurs at finite temperature. In this talk we present numerical results on the melting transition between the skyrmion lattice phase and the gas phase in a classical Heisenberg model-implementation of a chiral magnet. We particularly focus on the destruction of the bond-orientational and positional orders and discuss the connection to the two-dimensional melting in particle systems.

*Speaker

Effect of temperature specification on simulated ergodicity

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Temperature is an important ergodic function that is central to many computational research areas, such as condensed matter physics, chemistry, material science, molecular biology, nanotechnology and many others. The temperature specification used in a computation is crucially important, not least because all physical systems require temperature to clarify their state and stability. We discuss the apparent variability in temperature modeling and the effects of two common formalisms in molecular dynamics (MD) simulations. This variability is thought to affect the overall simulated ergodicity and therefore the structural evolution of the physical system. This question is not openly discussed in commercial simulation programs. We limit the comparison of the deterministic, ab-initio Newtonian and stochastic Monte-Carlo approaches to the equilibrium lattice face-centered cubic (fcc) constant to provide a meaningful comparison in the light of abundant literature data. The testbed is a collection of 1583 copper atoms in an isochoric system with the Sutton-Chen (SC) embedded atom model (EAM) as the interaction potential. The issues associated with either approach, particularly simulation accuracy, timescale, cooling and heating are investigated.

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Nucleation to percolation: crack growth in random spring ladder

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Crack growth and development are studied in a random spring ladder by molecular dynamics simulation. The springs have threshold for their displacements, assigned randomly from a uniform distribution. A spring snaps irreversibly once it is extended beyond its threshold value. The springs are Hookean and have angular potential associated with the angle between two adjacent springs. By increasing the angular force constant, we observe a transition in the development of fracture from the nucleation to percolation behavior. In the nucleation regime, a crack develops from the breaking of few consecutive springs and the crack grows till the entire ladder snaps. In the percolation regime, the breaking of the springs are uncorrelated and occurs randomly over the system. We also observe different avalanche behavior in the nucleation and the percolation regime. In particular, in the percolation regime, we observe power law avalanche behavior with power 5/2 that is predicted from the mean-field fibre bundle model. Our simulation results shows how different fracture patterns are obtained by tuning the elastic potential.

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Wang-Landau algorithm with the control of accuracy

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We propose modification of Wang-Landau algorithm for the direct estimation of the density of states. The previous versions of the algorithm are not able to give any idea on the convergence, and only can be tested for the models with the known density of states. We propose criteria of the convergences of the algorithm using information on properties of the random walk in the energy space. We give support of our proposal both analytically and numerically.

*Speaker

Non-canonical spin glass of polyhedral spin models on quasi-regular lattices

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Spin glass (SG) is an important subject in condensed matter physics and has long been a challenge for many optimization
algorithms in finding its grond state energy[1]. The so-called non-canonical spin glasses (SG's) with various spin models have recently attracted considerable attention [2,3,4,5,6]. This is a new type of SG system, different from the canonical one where both ferromagnetic (FM) and antiferromagnetic (AF) couplings exist. A non-canonical SG is a purely AF system having spins residing on a random connectivity lattice. The example of non-canonical SG's is the AF Ising model on a scale free network, which was first considered by Bartolozzi et al. [2]. A random connectivity lattice in the form of quasi-regular lattice can be obtained by randomly rewiring each site of a regular lattice to one or two of its next nearest neighbors. Accordingly, there exist abundance of triangular structures, whereby AF couplings lead the spins to be frustrated. The system therefore inhereted the main ingredients of spin glass, i.e., the randomness and frustration. As discreteness is important in phase transition, here we consider spin models with polyhedral symmetry, the underlining symmetry of such Platonic structures as cubic, icosahedron and dodecahedron. The counterpart model with continuous sysmmetry, the Heisenberg model, has been reported to exhibit no finite temperature SG phase [4,5,6]. By using Monte Carlo method with Replica Exchange Algorithm, we calculated the overlapping order parameter, which is a a commonly used quantity in searching for the existence of SG phase. Using finite scaling method, we estimate the critical exponents and temperatures of the observed SG phase transition.

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*Speaker

Improving and testing the population annealing Monte Carlo algorithm

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Population annealing is a promising recent approach for Monte Carlo simulations in statistical physics, in particular for the simulation of systems with complex free-energy landscapes. It is a hybrid method, combining importance sampling through Markov chains with elements of sequential Monte Carlo in the form of population control. In its established formulation, it appears to have algorithmic capabilities for the simulation of such systems that are roughly comparable to those of more established approaches such as parallel tempering, but it is intrinsically much more suitable for massively parallel computing. Besides presenting a highly efficient implementation of the algorithm for GPU devices, we present an upgrade of the method to a fully adaptive algorithm for the simulation of complex systems by an automatized choice of (1) the temperature step, (2) the time step, and (3) the population size. It is shown that in combination with the availability of a free-energy estimator, weighted averages and a multi-histograming technique the algorithm has the potential to successfuly tackle previously intractable problems and to become the approach of choice for a wide range of applications.

*Speaker

Synchronisation of Conservative Parallel Discrete Event Simulations in Small World Network

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We examine question of the influence of sparse long-range communications on the synchronisation in parallel discrete event simulations (PDES). We build a model for the evolution of local virtual times (LVT) in conservative algorithm, including three choices for the long-range communications. In all cases networks of links belong to the small-world network class. We found that synchronisation issue depends mostly on the average shortest path of the network, and clustering coefficient does not influent synchronisation. We found that critical exponent does depend on the fraction of the long-range links logarithmically. We present results of simulations and discuss our observations.

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Contour analysis of multi-affine nanostructure AZO thin films

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Morphology of aluminum-doped zinc oxide (AZO) thin films during spray pyrolysis growth has been characterized by two dimensional multifractal detrended fluctuation method and contour analysis. The results show that the investigated thin films are multifractal and multi-affinity strength increases with thickness enhancement. Contour analysis of these multi-affine structures show that the fractal dimension of a contour loop, D_f, for level cuts below and above the mean height has different values (in contrast to monofractal structures), while averaging it on all level cuts results in an identical $D_f = 1.13 \pm 0.02$, independent of samples thicknesses. Furthermore, there is a crossover to percolation regime with the exponent, $D_{f_p} = 1.42 \pm 0.02$. Fractal dimension of all contour loops, d, calculated by box-counting method, decreases with thickness enhancement, as the radius, length, and area of loops increase with thickness enhancement. The loops radius is linearly proportional to the grain size of deposited thin films and could be introduced as a new numerical parameter to determine this experimental measure.

*Speaker

Fluid Dynamics: from Macro- to Nano-fluidics

Design criteria for underwater superhydrophobicity: a rare-event molecular dynamics study.

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Superhydrophobicity refers to a set of remarkable macroscopic properties which a surface can show when it is wetted by a liquid. Such properties include the self-cleaning, anti-icing, anti-fouling, and the drag-reduction capabilities. In particular, drag reduction can be exploited in underwater applications to obtain high-performance marine vehicles with efficient fuel consumption or, to decrease energy consumption for liquid flows through tubes or channels.

In underwater conditions, superhydrophobicity and its properties stem from the presence of bubbles of vapor entrapped in the topography of the surface, this is the so-called Cassie state. However, such state is extremely fragile against pressure fluctuations which can lead to the complete wetting of the surface (Wenzel state), or to the cavitation (and growth) of a supercritical vapor bubble (pure vapor state). In the Wenzel and pure vapor states superhydrophobicity is lost.

In this work, inspired by the example of an underwater superhydrophobic fern[1]: the Salvinia molesta, we study the stability of the Cassie state for a surface with a nanoscale re-entrant topography with complex chemistry (hydrophilic top and hydrophobic interior) via rare-events molecular dynamics simulations. Rare-event methods allowed us to compute the free-energy barriers both for the Cassie-Wenzel, Cassie-pure vapor, and Wenzel-Cassie (recovery of superhydrophobicity) transitions at different pressure conditions. We found that the complex chemistry and the re-entrant topography improve the stability of the Cassie state [2] and allow the recovery of the superhydrophobic properties when the system is in the Wenzel state [3]. Starting from such findings, we developed simple design criteria for a more robust superhydrophobic surface in underwater conditions.

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*Speaker

Transient hydrodynamic finite size effects in simulations under periodic boundary conditions

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Microfluidic devices have drawn a lot of interest in biotechnology, where they can be used e.g. to separate platelets, white blood cells and red blood cells, or to detect macromolecules such as DNA. Nanopore-based and nanofluidic technologies seem to offer a good potential for high-throughput and affordable DNA sequencing [1] or for clean energy generation and water purification/desalination. Such applications involve complex flows under confinement, possibly with electrokinetic phenomena (coupled electrostatic and hydrodynamic effects). It is therefore important, in order to design setups or analyze experimental results, to be able to simulate such flows. Nevertheless, artefacts may arise due to the finite size of simulation boxes [2, 3]. In particular, Yeh and Hummer have shown that hydrodynamic effects lead to systematic size-dependent corrections to the diffusion coefficient (or mobility) in molecular simulations.
Here [4] we use the Lattice-Boltzmann method (LBM) [5] to investigate systematically the effect of the simulation box size and shape on the hydrodynamic flow generated by a point force in a bulk fluid (with an appopriate background compensating force), which corresponds to the Green's function for the Navier-Stokes equation. We show that the LBM is able to correctly predict the resulting finite-size correction on the mobility, both for cubic and anisotropic simulation boxes. In addition, we show that the results can be analyzed within the framework of linear-response theory to compute the velocity auto-correlation function (VACF) of a tracer particle. The long-time tail of the VACF predicted by hydrodynamic theory [6] is indeed observed for large simulation boxes, but is followed an exponential regime due to the finite box size. This demonstration of feasibility in bulk systems opens the way to the systematic study of finite-size effects on the mobility of confined fluids.

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Multiscale modelling of ion adsorption and electrokinetic phenomena in porous oxides.

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Porous oxides such as silica glasses or nonatitanates have numerous specific applications, especially in the domain of decontamination. Numerous elements can be exchanged or adsorbed in these systems. They are especially useful for nuclear decontamination because they relatively well resist to radiolysis. Despite their significance, theirs interfacial and electrokinetic properties are not very well understood. There is no consensus for the description of the interface. The various length scales involved make this class of systems especially challenging for computational physics.
We present a multiscale approach in order to describe ion separation and specific effects in porous oxides: silica glasses and nonatitanates. We will especially focus on electrokinetic phenomena. Extensive molecular simulations of aqueous electrolyte solutions confined in a charged amorphous silica slot have been performed. Generalyzing the McMillan-Mayer theory of electrolyte solution, the thermodynamical properties have been calculated in accordance with the experimental measurements.

For the dynamics, contrasting traditional models of the electric double layer, molecular dynamics simulations indicate that there is no stagnant layer, no Stern layer conduction, no outer Helmholtz layer. The description of the interface requires two points. First, a distinction has to be made between free and surface-bounded ions. The latter do not form a physical layer but rather a set of ion-surface contact pairs. Second, the mobility of the free ions relative to their bulk value is reduced. This effect proved to be from hydrodynamical origin needs to be included.

These two concepts, coupled to simple macroscopic equations, are sufficient to describe both equilibrium and electrokinetic (surface conductivity and electroosmotic flow) phenomena in agreement with the molecular simulations. The resulting macroscopic description is found to be valid up to very small porosities (typically 2 nm). Surface conduction is negative at high concentration, and the Bikerman formula is only valid at low concentration.

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Keynote: Hydration friction in nano-confinement: from bulk via interfacial to dry friction

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The viscous properties of confined water are relevant for many applications. Experiments measuring the friction between surfaces separated by thin water layers have suggested nano-confined water properties to differ drastically from bulk, but a microscopic picture of water-mediated nanoscale friction is missing. We study the shear friction between polar surfaces by non- equilibrium molecular dynamics simulations. With decreasing water film thickness we find three consecutive friction regimes: For thick films friction is governed by bulk water viscosity. At separations of about a nanometer the highly viscous interfacial water layers dominate and increase the surface friction, while at the transition to the dry friction limit interfacial slip sets in. We propose a confinement-dependent model that accounts for the additive friction contributions from bulk-like water, interfacial water layers and interfacial slip.

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Numerical investigation on spreading behavior of falling droplet on inclined surface

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Droplet impact on inclined surfaces is one of the frequently encountered phenomena which include raindrops, spray painting and coating. This is fundamentally an interesting problem as it involves various aspects of fluid mechanics together with inherent complexity. In order to explore the involved physics associated with the droplet dynamics, extensive analytical, experimental and numerical investigations have been reported by the researchers in the past few decades. El-Sherbini et al. [1] experimentally studied the motion of droplet on inclined surfaces and discussed the morphology of drops on various surfaces, for a range of inclinations and contact angles. A pioneering work in this field was carried out by by Brown et al. [2,3] who reported numerical formulations for droplets in contact with flat surfaces. Annapragada et al. [4] performed experiments and predicted the shape, contact area of droplets and advancing and receding contact angles of the droplet moving under gravitational acceleration as a function of droplet size and velocity. Recently, Jin et al. [5] experimentally investigated the impact and freezing processes of a water droplet for a range of inclination angles.

Although a plethora of investigations have been reported on falling droplets and its impact on inclined surfaces, these problems are considered separately in general. Spreading behavior of droplet after impact is also important and not explored in details especially on inclined surfaces. Moreover, it is important to investigate the effect of gravity which is neglected in most of the works reported so far. Accordingly, the aim of the present work is to investigate numerically the implications of droplet impact and inclination of the surface on spreading behavior of falling droplet. In this work, investigation of droplet dynamics with different inclination angles, based on the two-phase volume of fluid (VoF) model will be discussed. Temporal evolution of droplet on inclined surface with different inclination angles will be presented in detail in order to elucidate the spreading behavior of droplet.

Keywords: Falling droplet, Inclined surfaces, Droplet spreading.

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Solidification of a simple liquid near wall in high-speedl lubrication flows

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The Lennard-jones (LJ) fluid near the triple point under high-speed lubrications in parallel plate channel is investigated by molecular-dynamics simulations, where the temperature of LJ fluid is not controlled by any artificial thermostat algorithm but wall atoms are kept at a constant temperature. We find that the LJ fluid is solidified near the wall when the flow speed is sufficiently large even though the temperature of LJ fluid increases due to the viscous heating. We also find that a shear band appears in the solidified domain. This counter-intuitive phenomenon is explained in terms of the internal viscous heating in confined channel and is characterized by a non-dimensional parameter defined by the ratio of viscous heating to thermal conductivity. Furthermore the solidification near wall is little affected by the lattice structure of wall atoms but is a rather robust phenomenon occurring in the high-speed lubrications in confined channel.

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Molecular dynamics simulations of diffusio-osmotic flow driven by chemical potential gradient

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Osmotic transport driven by salinity difference or gradient is important and ubiquitous, occurring across many biological systems and used in various industrial applications. The recent interest in its applications to micro/nanofluidic devises, such as for desalination, energy harvesting, and biomedical technology, just to name a few, boosts the growth of this research field. In such diverse situations, one encounters the limitation of existing theoretical or numerical frameworks for studying the osmotic transports. In this context, we have recently proposed a new computational method for numerically studying the osmotic transport, as well as extended theories applicable to wider situations than existing ones. In this presentation, we report on molecular dynamics (MD) studies on osmotic transports. Main topic is focused on the diffusio-osmotic flow of a solute-solvent fluid adjacent to a solid surface, driven by a chemical potential gradient parallel to the surface. We propose a novel non-equilibrium MD (NEMD) methodology to simulate diffusion-osmosis, by imposing an external force on every particle, which properly mimics the chemical potential gradient on the solute in spite of the periodic boundary conditions. This NEMD method is validated theoretically on the basis of linear-response theory by matching the mobility with their Green-Kubo expressions. We apply the framework to more realistic systems, namely a water-ethanol mixture in contact with a silica or a graphene surface. In addition, we will also present some results of ongoing work on polymer structures in a solute-solvent fluid, under chemical potential gradients of solute particles.

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Chemical Physics

On the dynamics through a conical intersection

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Conical intersections represent critical topological features of potential energy surfaces and open ultrafast nonradiative deactivation channels for photoexcited molecules. In this talk, I will present how this funneling picture is transposed in the eyes of the exact factorization formalism [1]. The exact factorization of the total molecular wave function [2] leads to the fundamental concept of time-dependent potential energy surface and time-dependent vector potential [3], whose behavior during a dynamics through a conical intersection has only recently been explored [1]. Despite the fact that these quantities might be viewed as time-dependent generalizations of the adiabatic potential energy surfaces and the nonadiabatic coupling vectors, characteristic quantities appearing in the Born-Oppenheimer framework, we observe that they do not exhibit particular topological features in the region of the conical intersection but still reflect the complex dynamics of the nuclear wavepacket.

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*Speaker

Interlayer binding of bilayer blue phosphorus: quantum Monte Carlo study

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Both quantum Monte Carlo (QMC) and density functional theory (DFT) calculations have been performed to investigate accurate ground-state properties of blue phosphorus, one of the stable layered phosphorus allotropes with a puckered honeycomb structure. We first find that the DFT significantly overestimates the cohesive energy of single-layer blue phosphorus when compared to the QMC, indicating some limitations of DFT calculations in describing sp3 covalent bonding of phosphorus atoms. In the study of bilayer blue phosphorus, the AA stacking mode turns out to be energetically favored by 10 meV/atom over the AB one. In addition, the comparison of our QMC results with the DFT ones based on several different van der Waals (vdW) exchange-correlation functionals suggests that the interlayer binding in bilayer blue phosphorus may not be purely described by the vdW interaction. From the fact that some excessive charges are accumulated in the middle between the phosphorous layers at their dissociation limit, we conclude that additional chemical bonding other than the vdW interaction is involved in their interlayer binding.

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Estimating thermodynamic expectations and free energies in expanded ensemble simulations: systematic variance reduction through conditioning

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Markov chain Monte Carlo methods are primarily used for sampling from a given probability distribution and estimating multi-dimensional integrals based on the information contained in the generated samples. Whenever it is possible, more accurate estimates are obtained by combining Monte Carlo integration and integration by numerical quadrature along particular coordinates. We show that this variance reduction technique, referred to as conditioning in probability theory, can be advantageously implemented in *expanded ensemble* simulations. These simulations aim at estimating thermodynamic expectations as a function of an external parameter that is sampled like an additional coordinate. Conditioning therein entails integrating along the external coordinate by numerical quadrature. We prove variance reduction with respect to alternative standard estimators and demonstrate the practical efficiency of the technique by estimating free energies and characterizing a structural phase transition between two solid phases.

*Speaker

Nuclear quantum effects in molecular dynamics simulations

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To take into account nuclear quantum effects on the dynamics of atoms, the path integral molecular dynamics (PIMD) method [1] used since 1980s is based on the formalism developed by R. Feynman. However, the huge computation time required for the PIMD reduces its range of applicability, in particular at low temperature and when using a first-principles description of the interatomic forces. Another drawback is the requirement of additional techniques to access time correlation functions (ring polymer MD or centroid MD).
We developed an alternative technique based on a quantum thermal bath (QTB) [2,3] which reduces the computation time by a factor of _˜20. The QTB approach consists in a classical Langevin dynamics in which the white noise random force is replaced by a Gaussian random force having the power spectral density given by the quantum fluctuation-dissipation theorem. The method has yielded satisfactory results for weakly anharmonic systems. The QTB satisfactorily describes, in particular, the quantum harmonic ascilator, the heat capacity of a MgO crystal, and the isotope effects in LiH and LiD.
Unfortunately, QTB is subject to the problem of zero-point energy leakage (ZPEL) in highly anharmonic systems, which is inherent in the use of classical mechanics. Indeed, a part of the energy of the high-frequency modes is transferred to the low-frequency modes leading to a wrong energy distribution. We have shown that in order to reduce or even eliminate ZPEL, it is sufficient to increase the value of the frictional coefficient [4]. For example, the complete sequence of ferroelectric phase-transitions in the BaTiO3 perovskite are reproduced at the correct temperatures.
Another way to solve the ZPEL problem is to combine the QTB and PIMD techniques [5]. It requires the modification of the power spectral density of the random force within the QTB. This combination can also be seen as a way to speed up the PIMD. Unfortunately, as in PIMD, the major disadvantage is that time-dependent correlation functions are not directly accessible.

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Simplifying calculations of IR and Raman spectra from DFT-based molecular dynamics simulations

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We present our recent work on the simplification of the calculation of IR and Raman spectra from DFT-based molecular dynamics simulations (DFT-MD). In order to calculate these spectra from DFT-MD, one has to Fourier transform the time-correlation function of the dipole moment (IR) or polarisability tensor (Raman) of the investigated system. Calculating such dipole or polarisability tensor has a computational cost, which is very expensive especially in complex condensed matter systems such as liquids. It is especially crucial when one is interested in the IR/Raman spectrum of solute(s) immersed in liquid (water for instance), as one does not want to get the IR/Raman spectrum of the whole system, which would be the default route if one calculates the dipole/polarisability tensor of the simulation box. On the contrary one wants to evaluate the dipole/polarisability tensor of each single molecule of the system, and thus extract the IR/Raman spectrum only of chosen molecules within the whole system (typically the solute(s)). This requires apply a localization procedure of the wavefunction of the whole system (the only entity known) onto each molecule of the liquid at each time step of the trajectory. This can now routinely be done through e.g. a Wannier localization procedure. This is however computationally costly to achieve at each time-step of the dynamics, and the cost can be estimated as roughly doubling/tripling the computational cost of the trajectory. We have developed a method to avoid such computational cost and instead rely on Fourier transforms of time-correlation functions of velocities, weighted by well-chosen observables. Velocities being natural variables from the dynamics, these Fourier transforms are computationally calculated for free. Observables such as APT tensors for IR spectroscopy have been chosen for the necessary weights/pre-factors. We will present our methodology, and will demonstrate how it works for molecules (of increasing complexity and flexibility) in the gas phase, and how good the IR spectra can be in comparison to the exact calculation. We will then show the extension of the method to IR spectroscopy of complex systems, i.e. spectroscopy of solute(s) immersed in liquid water.

*Speaker

Improving Solubility in Supercritical CO2: Theoretical Studies of CO2-philic Compounds and Solubilizers

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The peculiar properties of fluids in the supercritical phase have motivated remarkable advances in the domain of Chemical Physics. Indeed, the molecular factors leading to a very large compressibility of the fluid near the critical point, the presence of long scale correlations in the density fluctuations and, in same cases, the appearance of local density augmentations represent real challenges for fundamental research. Moreover, the thermodynamic control that can be easily achieved on the system has made supercritical fluids appealing for the development of new technologies. In particular, supercritical carbon dioxide (scCO2) is a nontoxic, easy to obtain and to recycle medium for which the supercritical conditions are readily obtained from an experimental point of view. Although its extensive use for industrial application, for separation and extraction (*e.g.*, coffee decaffeination), a major bottleneck exists to further progress: the low solvation strength of CO2 with respect to large molecular species and polar compounds.
Important steps forward to overcome this issue have been made thanks to the use of cosolvents and microemulsions. The most important discoveries, however, concern the use of the concept of CO2-philicity, leading to the design of systems containing atoms or groups displaying specific interactions with CO2. The work that has been recently carried out in our group has focused on this particular point. By using *ab initio* calculations on model systems, we have characterized the nature of the interaction making carbonyl compounds CO2-philic and provided some routes to enhance this property. This knowledge has inspired the search for systems that might act as *solubilizers* in scCO2, such as macromolecular systems that can encapsulate nonsoluble molecules and drive them in the supercritical medium. By analogy with the aqueous systems, we proposed the use of β-cyclodextrins as supports for host-guest binding in scCO2. In collaboration with experimentalists, this has allowed us to design, synthetize and characterize the first stable inclusion complex formed in an acetylated β-cyclodextrin in scCO2, opening the door to a larger use of the concept of solubilizers and possibly to supramolecular Chemistry in this supercritical medium.

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All-trans, all-cis and mixed isomers of azobenzene star: A multiscale simulation study

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The main property of azobenzene (azo) is its fully reversible photoisomerisation reaction, which changes the molecule from the flat trans-state to the non-planar cis-state. This affects the dipole moment and the excluded volume of the molecule. Azobenzene can therefore act as a molecular switch that responds to UV-vis light: It is known that in more complex systems, e.g. when azobenzene is embedded in a polymer matrix or when a molecule contains multiple azo-groups, the photoisomerization can induce macroscopic deformations or influences the self-assembly of such macromolecules [1]. Azo-containing materials are therefore highly promising for applications ranging from data storage to artificial muscles and optical devices.
We present multiscale (DFT and MD) simulations of a star-shaped molecule consisting of a benzene-1,3,5-tricarboxamide core and three azobenzene groups, which are symmetrically attached to the central ring. The star therefore constitutes a multichromophoric system. Each arm can undergo the photoisomerisation reaction and thus the molecule exhibits four photoisomers: ttt (all-trans), ccc (all-cis) and two mixed states (ttc and tcc).

Using Gaussian 09 Rev A0 [2] and B3LYP/6-31G(d,p) functional [3] we optimize these geometries and investigate the structural and optical properties of each state. Specifically, we intend to identify the influence of connectivity between the multiple azo-groups on these characteristics.

Furthermore, using all-atomistic molecular dynamics (MD) simulations we investigate the behavior of a single molecule and the collective behavior in aqueous solution. We model the molecules within PCFF (Polymer Consistent Force Field) [5] and the simulation package Lammps [4]. First of all, the hydration properties of different isomers are investigated by applying the thermodynamic integration method. When not exposed to light, i.e. all arms are in trans-state, the multichromophores assemble in columnar structures. In line with experiments [6], the simulations show that these H-aggregates are formed due to π-π-stacking between the central rings and H-bonding between amide groups. Here, we additionally characterize the cluster size, shape and the stability of aggregates. In another case, the system is exposed to light, meaning that the azobenzene groups undergo the trans-cis photoisomerisation. This effect is modeled by an ad-hoc modification of the dihedral potential that encompasses the azo-bond (N=N double bond). It is then examined how the clusters are affected and how the system reorganizes.

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Open Boundary / Grand-Canonical Adaptive Resolution Simulations of Ionic Liquids

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We extend the use of the adaptive resolution (AdResS) method in its grand canonical-like version (GC-AdResS) to the molecular dynamics simulation of a large class of IL's. We show that the partitioning of the total system in a subsystem of interest with atomistic details and a reservoir of coarse-grained particles leads to satisfactory results. The challenging aspect of this study, compared to previous AdResS simulations, is the presence of charged particles and the necessity of addressing the question about the minimal physical input needed to model the coarse-grained particles in the reservoir. We propose two different approaches (see figure above) and show that in both cases they are sufficient to capture the decisive physical characteristics that allow a valid system–reservoir coupling. The technically satisfactory results pave the way for the multiscale analysis of ionic liquids and truly open boundary molecular simulations. GC-AdResS is then employed as a tool for identifying the essential atomistic degrees of freedom required for structural properties with different degree of locality in space and time; the previous analysis allows for a genuine understanding of the multiscale characteristics of IL's.

*Speaker

Vibrational energy relaxation at water interfaces from ab initio molecular dynamics simulations

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Ab initio molecular dynamics simulations represent a versatile approach to investigate the structure and dynamics of water interfaces, especially in the cases of heterogeneous systems where less computationally demanding techniques, such as force field approaches are not easily transferable. Recently, *ab initio* simulations have been used to calculate Sum Frequency Generation spectra, also thanks to new developments in the calculations of the response functions, which make use of velocity-velocity correlation functions incorporating the appropriate selection rules [1,2].
We present here a new approach to investigate vibrational energy relaxation at water interfaces from the analysis of *ab initio* molecular dynamics trajectories. We follow the energy relaxation from a locally excited vibrational state using suitable descriptors based on vibrational density of states.

Our method is applied to different water systems, including bulk water and fluorite/water interfaces at different pH. In the case of the fluorite/water interface at low pH we find that water behaves similarly to bulk water, while, in the case of high pH, instead, the energy relaxation is much slower. A molecular interpretation of the different time scales is provided.

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Free energies of solvation and binding, and solvent positions around any molecule in few minutes by rigorous liquid state theories

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Solvation of molecules and macromolecules, protein-drug affinity, electrode-solvent interfacial properties, colloidal interaction... are driven by physical phenomena at the sub-nanometer range. Understanding them correctly requires an explicit description of the solvent molecules at the same microscopic level as the solute itself. As an alternative to the precise but very time consuming explicit solvent numerical simulations, we propose a liquid-state physics approach based on the molecular Ornstein-Zernike equation, the integral equations (IE) and the classical density functional theory in three dimensions (3D-DFT). Using powerful algorithms for the angular representation of the solvent molecules, optimized numerical codes and higher order IE or DFT, we will show how to compute *in a few minutes* accurately the solvent position and orientation distribution around a given solute or between two solutes and the associated free energy of solvation or binding.

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Hidden Beneath the Surface: Origin of the Observed Enantioselective Adsorption on PdGa(111)

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The PdGa intermetallic compound emerged recently for its remarkable catalytic properties in the purification of the feedstock for polyethylene production. PdGa has an intrinsically chiral structure, with subtle structural differences at the {111} surfaces of the two enantiomers. Recent experimental observations in our laboratory [1] reveal a striking enantioselectivity of the PdGa:A(111) (resulting in exceptionally high enantiomeric excess ratios of up to 98%, and confirmed by analogous adsorption experiments on the complementary enantiomer) with respect to adsorption of the prochiral molecule 9-ethynylphenanthrene. The findings highlight the great potential of intrinsically chiral intermetallic compounds for the development of novel, enantioselective catalysts that can be operated at high temperatures and potentially also in harsh chemical environments. The question arises why does the bulk chirality of PdGa result in such a dramatic selectivity. We investigate this phenomenon using density functional theory calculations. It results that the key ingredient to understand the experimental evidence is the appropriate description of van der Waals interactions: whereas simplified schemes based on nucleus-centered phenomenological contributions as well as schemes including non-local vdW corrections do not explain the adsorption energy difference between the two enantiomeric configurations, an approach [2,3] based on the calculation of the dielectric function in the substrate material (MBDsurf) appropriately weights the long-range interactions leading to a result compatible with the measurements reported in the literature.

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*Speaker

Keynote: Rare Events Methods, Reaction Coordinates, and Useful Rate Theories

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Among the growing arsenal of rare events methods and reaction rate theories, three antiques stand out for their extraordinary capabilities. Specifically, these are harmonic transition state theory, classical nucleation theory, and Marcus theory. For bond breaking/making reactions, nucleation, and electron transfer, these three theories remain the central conceptual frameworks behind countless computational methods. They are unrivaled in their ability to predict kinetic trends as a function of temperature, supersaturation, electrochemical potential, and many other properties. They even provide the theoretical justification for free energy relationships that predict kinetic trends across series of related reactions. The capabilities of these three classic theories derive from a shared feature at their foundations: each was built around a scalar reaction coordinate which has a clear physical meaning and is also generalizable across many reactions, nucleation processes, and electron transfer processes, respectively. By comparison, modern computational frameworks that directly use abstract reaction coordinates (e.g. committors or eigenfunctions from diffusion maps or Markov state models) invest a massive simulation effort to generate one rate at one condition. It remains difficult to extract mechanistic insight from these abstract reaction coordinates. Taking the three classic theories as a guide, I ask how we might discover similarly generalizable reaction coordinates and useful theories for those activated processes that as yet remain poorly understood. I will demonstrate our recent progress toward this goal using likelihood maximization approaches.

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SFG spectroscopy of Silica/water interfaces by DFT-MD simulations

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We will present recent DFT-MD simulations of electrolytic silica/water interfaces (electrolytes are KCl, NaCl, NaI) in order to unravel the structural properties of electrolytes at the crystalline quartz/liquid water interface and at the amorphous silica/liquid water interface, including pH effects, and how water and surface both modulate each other response to the presence of electrolytes. The theoretical method employed to calculate SFG spectra from DFT-MD simualtions is presented. A detailed analysis of the non-linear SFG spectral signatures of the investigated electrolytic silica/water interfaces is presented, comparisons between the different mineral/water interfaces allow us to definitely conclude on how the structural arrangements of liquid water at these electrolytic interfaces modulate the final spectroscopic signatures.

*Speaker

Ab initio molecular dynamics simulations of RNA nucleotides in hydrothermal prebiotic environment

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According to the RNA world hypothesis, self-replicating ribonucleic acid molecules may have been precursors to current life on Earth, due to its wide versatility in different biochemical processes. Previous experimental studies have explored how the RNA synthesis have occurred in plausible prebiotic conditions, comprising the catalytic role of mineral surfaces, the presence of salts or lipid compounds, the exposure to drying/wetting cycles, and so forth [1]. In this regard, one of the main challenges is the formation of RNA monomers, named, nucleotides, that subsequently reacted to form more complex RNA oligomers.

In this study, we provide quantitative new insights on the chemical reactions of RNA nucleotides under hydrothermal prebiotic conditions, by means of Born-Oppenheimer molecular dynamics simulations in explicit solvent. Moreover, we also exploit enhanced sampling techniques such as metadynamics [2] and umbrella sampling [3] in combination with a topological approach developed in our team that accurately tracks the changes in the chemical bond network along a reaction [4]. From this metodology, we are able to explore different reaction pathways related with the nucleotide formation as well as quantitatively obtain the free energy profiles. In addition, we explore the nucleotide phosphorylation considering hydrothermal and standard environments to get further information about

*Speaker

the chemical mechanism and its thermodynamics and to understand the role of such an important exothermic reaction during prebiotic evolution.

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Keynote: Modelling Supramolecular Polymers

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Molecules interacting via weak, noncovalent, reversible interactions can aggregate in solution along one or more dimensions to form supramolecular polymers. The mechanism of their self-assembly proceeds via either of two mechanisms: cooperative or isodesmic which can be differentiated through the association constant (K) between the molecules. In the former, K depends on the length of the oligomer while it is independent of the oligomer size for an isodesmic growth. Recent advances in this field have enabled big applications in optoelectronics, solar cells, light harvesting etc. Supramolecular polymerization also aids in our understanding of assemblies in biology.
Atomistic and coarse grained molecular dynamics simulations on chemically specific models enable us to understand the microscopic processes, thermodynamics, structure and dynamics in supramolecular polymerization. Illustrative examples from well studied systems, Benzene-1,3,5-tricarboxamide (BTA) and perylene bisimides (PBI) will be presented. It is shown that the presence of motifs in the molecule which leads to a long range interaction along the stacking direction leads to a cooperative growth of the polymer. Furthermore, the application of an external electric field on the liquid crystalline phase of a C3 symmetric supramolecular system exhibits not only a reversal of polarization, but also that of the handedness of the stack.

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Analysis of local bond-orientational order for liquid gallium at ambient pressure

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The static structure factor (SSF) of liquid Ga at ambient pressure (AP) has been observed for nearly half a century and is well known for exhibiting a shoulder on the high-q side of its first peak [1]. However, resolving its local structure for producing the high-q shoulder remains a subtle problem in liquid metal researches. In the present work, we investigated local structures of liquid Ga via *ab initio* molecular dynamics (AIMD) simulations by using the VASP code for 1331 Ga atoms at AP and 323 K, just above the melting temperature ($Tm = 302$ K).
In terms of the local bond-orientational order (LBOO) parameters, a cluster approach for analyzing local structures of atomic liquids was developed [2]. In this approach, a cluster in a liquid is defined as a combination of neighboring seeds and their nearest neighbors, where seeds are particles having at least *nb* local-orientational bonds, and a cluster ensemble is a collection of clusters that are specified with LBOO *nb* and number of seeds. Both q4 and q6 LBOO parameters were used to analyze structures of the liquid generated by the AIMD simulation. In generated configurations, particles with low coordination numbers had a preference for local structures exhibiting fourfold orientational symmetry. Further, two types of cluster structures were found in the simulated liquid, with one characterized by sixfold orientational symmetry and the other typified with fourfold orientational symmetry. Cluster ensembles with sixfold orientational symmetry displayed SSFs akin to that of a hard-sphere fluid. On the contrary, the SSFs of cluster ensembles with fourfold orientational symmetry behaved similarly as the anomalous SSF of liquid Ga by exhibiting an asymmetry in the first peak or even a high-q shoulder.

We also examined the similarity between local structures in the simulated liquid and the structures of Ga solids, including a-Ga, b-Ga, Ga II and Ga III. In the (q4, q6) map, the points of these Ga solids were located on the rim of the distribution of the liquid. In addition, a highly LBOO cluster whose SSF displayed a high-q shoulder had local structures more similar to β-Ga than other Ga solids. Furthermore, the structures of cluster ensembles with fourfold orientational symmetry were found to resemble more to the structure of β-Ga.

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*Speaker

Soft Matter and Biophysics

Conformational dynamics of the human Guanylate binding protein 1 from Hamiltonian replica exchange MD simulations and FRET experiments

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Guanosine triphosphate (GTP) binding proteins (GBPs) play essential roles in many cellular processes responsible for the maintenance and regulation of biological functions. They are a large family of enzymes that can bind and hydrolyze GTP resulting in a wide range of GTPase activities depending on the individual task of the protein. The human GBP 1 (hGPB1) was found to be involved in antiviral and antibacterial defense but was also identified as a marker of various cancer types, such as mammary cancer. After GTP binding and hydrolysis, substantial structural changes occur in the GBP proteins with bound nucleotide. Thus, GBPs can adopt at least two structural states that can lead to different binding affinities to partner proteins and the GTP bound state is able to form dimers thought to be the smallest assembly able to perform the biological function of the protein. Even with the resolved crystal structure of the hGBP1 monomer, the structural dynamics of the apo conformation in solution and its impact on the GTP binding and protein dimerization is not well understood.

Here we employ enhanced sampling Hamiltonian replica exchange MD simulations of the hGBP1 protein in explicit solvent to investigate the conformational ensemble and dynamics explored by this protein in its monomeric apo form. The conformational states sampled in the simulations are corroborated with data from F´orster resonance energy transfer (FRET) experiments. By using fluorescence labels at two different locations/amino acids of the protein, FRET experiments are able to identify distances between the two labels associated with different conformational states as well as relaxation times that correspond to the identified states. Such experiments were performed for twelve pairs of amino acids of hGBP1. The distances associated with the fluorescence labels are also derived from the MD simulations performed here and the conformational states and motions from MD simulations are combined with the experimental FRET results for a complete description of the apo hGBP1 conformational dynamics in solution.

*Speaker

Electron Transfer in Organic and Biological Materials

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Charge transfer processes are ubiquitous and play a prominent role in biology and material science. While experiments give valuable information on certain kinetic and thermodynamic properties of charge transfer events, they usually do not offer a molecular-level insight into these phenomena. Adequate simulations can bridge the gap between microscopic processes and macroscopic charge transports. For instance, a combination of Marcus theory, classical molecular simulation and master equation formalism can estimate complex charge transfer processes involving multiple redox sites in large systems [1]. But such rate-based approaches usually only work for localized charge carriers and in situations where the charge transfer is a rare event in the time scale of other molecular motions. To surpass these limitations, we have recently implemented a fast non-adiabatic molecular dynamics approach (based on Tully's surface hopping) where the wavefunction of the charge carrier is explicitly propagated in the time-dependent potential created by (classical) nuclear motion [2,3]. First applications to hole transfer in the ethylene dimer successfully reproduced exact results from the theory [3] and applications to a chain of ethylene molecules successfully predicted a crossover from activated to band-like transport [2]. Here we present a new implementation of the method into the CP2K software that enables us to model fast charge transfer in larger, application relevant organic crystals consisting of thousands of atoms. We will present applications as well as a detailed analysis of the charge transfer mechanism predicted by our surface hopping approach.

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Keynote: Molecular simulations of membrane sensing and remodeling

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Living cells need to exert tight control over their lipid membranes to maintain their internal structure, to guard their outside boundary, to establish potential and concentration gradients as their energy source, or to transmit signals between their compartments and to the outside. As a consequence, elaborate protein machineries have evolved that allow cells to sense and regulate both shapes and physical characteristics of their lipid membranes. The molecular modeling of these machineries faces significant challenges because of their complexity, size, and dynamic nature. To address these challenges, we combine atomistic and coarse-grained simulations of protein-membrane systems. In my talk, I will describe different mechanisms used by eukaryotic cells to sense and regulate the fluidity of their lipid membranes, as deduced from molecular dynamics simulations and experiments. In addition, I will use simulations to explore large-scale membrane remodeling processes, from vesicle fusion to the shaping of organelles. To highlight one of the technical challenges, I will discuss the unusual hydrodynamics in simulations of quasi-2D membranes under periodic boundary conditions.

*Speaker

Finding protein folding funnels in random networks

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Many attempts have been made for understanding protein folding dynamics using network representations of folding pathway. For example, the Markov state model has been widely used for expressing the transitions between protein conformations in folding trajectories obtained by molecular dynamics simulations. In the present work, I, too, focus on the network structures of protein folding dynamics, but from a somewhat different perspective. Currently most widely accepted theoretical framework of the protein folding is so-called the funnel picture, which states that the number of conformations decreases as the energy lowers from the denatured state towards the native state. In other words, the energy landscapes of proteins have been designed through Darwinian evolution, so that proteins readily fold to their native states. A question I would like to ask here is "How rare are such folding-friendly funnel structures?".
As a first attempt to answer this question, I introduce a random network model with each nodes assigned a random energy. Nodes represent the metastable conformation ensembles. One of the nodes is considered as the denatured state and another the folded state. Other nodes represent the intermediate conformation ensembles between them. The edges connecting the nodes are possible transitions between the nodes. The network structure is assumed to be determined by the conformation of the native state, and the energy assignment is considered to reflect the amino-acid sequence. I then define the ideal funnel structure for this model as follows: Starting from the denatured state, if all the paths connecting the nodes in energy-lowering direction lead to the folded state, then the network is regarded to have an ideal funnel structure.

The task now is to compute the probability that the ideal funnel is realized for a given network by changing the assignment of energy. Since we need only to know which node has lower energy for each edge, integer numbers are assigned which express the order of energies to the nodes instead of the values of energies. Then what we have to do is to count the number of arrangements of these integers that make the ideal funnel. In order to count such arrangements statistically, I employ the Multi-Canonical Monte Carlo method with the weights being determined by the Wang-Landau procedure, which we have already used to estimate the number of magic squares[1].

I generated 1000 networks randomly for networks of the size up to 27 nodes and estimated the probability of ideal funnels for each size. It was found that the probability is widely distributed from network to network, and close to the log-normal distribution . This result implies that there are a small number of networks that are robust against the mutation. It may relate to the fact that the number of the existing folds is not so large. The funnel structure becomes rarer exponentially as the

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protein becomes longer. The robust networks also decreases exponentially, but significantly slower than the typical networks. That is also an advantage in evolution, because the number of the robust networks decreases relatively slowly.

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Weak Nanoscale Chaos And Anomalous Relaxation in DNA

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Anomalous non-exponential relaxation in hydrated biomolecules is commonly attributed to the complexity of the free-energy landscapes, similarly to polymers and glasses. It was found recently that the hydrogen-bond breathing of terminal DNA base pairs exhibits a slow power-law relaxation attributable to weak Hamiltonian chaos, with parameters similar to experimental data (PRL, 115, 188104, 2015). We study the relationship between this motion and spectroscopic signals measured in DNA with a small molecular photoprobe inserted into the base-pair stack. To this end, the earlier computational approach is applied to the experimental DNA fragment. The intensity of breathing dynamics is strongly increased in the internal base pairs that flank the photoprobe, with anomalous relaxation quantitatively close to that in terminal base pairs. The possible physical mechanism of the coupling between the relaxation of base-pair breathing and the experimental response signal involves an interplay between the solvent and DNA dynamics. It is concluded that the algebraic relaxation observed experimentally is very likely a manifestation of weakly chaotic dynamics of hydrogen-bond breathing in the base pairs stacked to the photoprobe, and that the weak nanoscale chaos can represent an ubiquitous hidden source of non-exponential relaxation in ultrafast spectroscopy.

*Speaker

Viscoelastic hydrodynamic interactions and anomalous CM diffusion in polymer melts: influence of thermostat and simulation box

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We have recently discovered that anomalous center-of-mass (CM) diffusion occurring on intermediate time scales in polymer melts can be explained by the interplay of viscoelastic and hydrodynamic interactions (VHI). The theory has been solved for unentangled melts in 3D [1] and 2D [2] and excellent agreement between theory and simulation is found.
The physical mechanism considers that hydrodynamic interactions are time dependent because of increasing viscosity before the terminal relaxation time; it is generally active in melts of any topology. Surprisingly, the effects are relevant for both, momentum-conserving and Langevin dynamics [1,2] and this presentation will focus on the differences: The commonly employed Langevin thermostat significantly changes the CM motion on short and intermediate time scales, but approaching the Rouse time, the melt behavior is close to momentum-conserving simulations. On the other hand, if momentum-conserving simulations are run in too small a simulation box, the result looks as if a Langevin thermostat was used. Finally we will comment on the crossover from 2d to 3d in thin film confinement where we have given a new quantitative estimate of the entanglement density as a function of film thickness [3]. (1) J. Farago, H. Meyer, A.N. Semenov PRL 107, 178301 (2011); PRE 85, 051807 (2012).
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*Speaker

Transition to network synchronization in neuronal cultures: modelling the activity bursts with an adaptive 2D dynamical model

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Synchronized periodic bursts of activity emerge spontaneously in *in vitro* neuronal cultures under physiologic conditions [1]. Such a network bursting is characterized by an intermittent collective neuronal activity [2,3] in which long quiet periods – with almost no spike emission – are followed by short periods of intense spiking where the whole network displays high firing rates. Experimentally, the transition from an unsynchronized state where a large majority of neurons oscillate independently to a synchronized collective one where the population exhibits network bursts can be triggered by the extracellular calcium concentration accounting for synaptic strength [1]. We carry out a modelling of these phenomena where the behavior of each neuronal potential is described with the help of a 2D dynamical system, and the adaptation by a slow variable which couples the two differential equations (Adaptive Exponential Integrate and Fire model [4]). The coupling between neurons all over a directed network occurs through a representation of synapses by 'alpha' functions [$k/\mathrm{t}\ \exp(-t/\mathrm{t})$] . Our simulations aim at being as close as possible to experiments where networks comprise up to 100 000 neurons each of them coupled to other ones through several tens of synapses. These simulations are carried out with the help of the neuron simulator 'NEST' implemented on a massively parallel Blue Gene supercomputer. We focus on the description of the dynamical attractor to which the population converges when the synaptic coupling increases [5]. We show that a sufficient condition for bursting to occur is the presence of an excitatory population of oscillatory neurons displaying spike adaptation and a strong enough synaptic coupling k. Addition of inhibitory neurons or plastic synapses can then modulate this dynamics in many ways but is not necessary for its appearance. After discussing the origin of the bursting behavior, we provide a detailed analytic and numerical description of such dynamics, as well as the evolution of its properties depending on the neuronal

*Speaker

and synaptic parameters.

Theoretical studies on stability and dynamics of protein complex by a coarse-grained model

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Plastocyanin(PC) is one of type I copper proteins which have one copper ion in their active site and has the function of electron transfer between proteins. In photosynthesis, PC transfers one electron from cytochrome f(Cytf) in cytochrome b6f complex to P700 in Photosystem I. PC is diffusing between Cytf and P700 in the lumen side of the thylakoid membrane. In order to investigate both association process and diffusion process of PC, it is a tool to simulate large size systems including many proteins on long time scale by using coarse-grained models. In our pervious study, we have presented a coarse-grained model including intermolecular interactions consisting of hydrophobic interaction between proteins. In this study, we extend the simple coarse-grained model for describing intermolecular interaction between proteins in solvent to investigate the association, self-assembly behaviour. The new expression of the hydrophobic potential is presented in similar way to the concept of molecular-crowding effects. We discuss the association process of type I copper proteins PC-Cytf by using our simple coarse-grained model in relation to the binding modes between interacting proteins and to the free energy landscape of the complex.

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Protein adaptation to high temperatures does not necessary require enhanced mechanical stability

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Because thermophilic proteins are stable and functional at high temperature but generally lack activity under ambient conditions, it has been suggested that thermal stability was associated with enhanced mechanical rigidity [1]. Single-molecule force-spectroscopy techniques appear as a natural tool to inquire the correlation between protein thermal and mechanical stabilities. Using an original approach combining their *in silico* variant, steered molecular dynamics, and atomistic Hamiltonian-replica exchange simulations at an all-atom resolution in explicit solvent to study two homologues of the cold-shock protein family, we unambiguously show that thermal and mechanical stabilities are not necessarily related. Indeed, both the mesophilic and the thermophilic homologs offer moderate resistance to mechanical force. The mesophilic protein is even found to be more resistant, because of the confirmation of a large loop that hinders unfolding along the pulling direction. The simulated protein melting curves are obtained using a computationally effective and original replica-exchange simulation scheme [2]. We recently pioneered the use of this technique to assess protein thermal stability [3], and we show here that the obtained melting curves are in very good agreement with experimental data, reinforcing the validity of our approach that can identify the protein "weak" spots for mechanical and thermal unfolding, which are found to be distinct.

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Mesoscale Hydrodynamic Simulation of Microswimmers

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Multiparticle collision dynamics (MPC), a particle-based mesoscale simulation technique for fluids, has been developed into one of the major simulation techniques for complex fluids during the last decade. MPC captures thermal fluctuations and is easily coupled with, e.g., molecular dynamics simulations for embedded objects [1]. We have analyzed its hydrodynamic properties [2] and investigated the nonequilibrium dynamics of various microswimmers [3-6]. In this contribution, we will present simulation results for the swimming motion of *E.coli* bacteria in bulk and at interfaces [7]. We find that *E.coli* senses the nanoscale slip length of the surface and responds with a circular trajectory of a particular radius. The obtained dependence of the curvature on the slip length is well described by a simple theoretical expression. Moreover, we employ these insights to suggest a novel route to direct bacterial motion. In addition, the swimming dynamics of spheroidal squirmers will be discussed in a slit geometry [8]. Here, we find that pullers exhibit a cooperative motion stabilized by surface-hydrodynamic interactions. Considering the collective behavior, we find that hydrodynamic interactions suppress motility-induced phase separation (MIPS) for spherical squirmers. In contrast, hydrodynamics enhances MIPS for spheroidal squirmers.

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*Speaker

Monte Carlo simulation for pattern formation of run-and-tumble chemotactic bacteria

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We investigate the instability and pattern formation in a kinetic transport equation for the chemotactic bacteria coupled with a reaction-diffusion equation for the chemoattractant. On the theoretical side we obtain a linear instability condition, in which a stationary homogeneous state in the population density becomes linearly unstable when the stiffness of chemotaxis is sufficiently large and then stationary periodic patterns are generated. A remarkable property is that the unstable frequencies remain bounded, as it is the case in Turing instability. We perform the Monte Carlo simulations for the initially homogeneous state with changing the parameters involved in the linear instability condition. The numerical results demonstrate that the obtained instability condition is compatible and even sharply prescribe the occurrence of the linear instability and pattern formation.

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The challenge for Gram-negative bacteria: Towards in-silico screening of antibiotics for fast permeation through nanopores

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The demand of new drugs for combating multidrug-resistant bacteria appears more urgent for Gram-negative bacteria: the presence of the outer membrane, which hinders the access of molecules to internal targets, renders the development of anti-infectives more challenging. Today neither a robust screening method for permeation nor defined physical/chemical rules governing permeation through the outer membrane are available. The main path for polar molecules to overcome the outer membrane is constituted by hour-glass shaped nanochannels known as porins. By assuming diffusion as the physical mechanism of the transport of molecules through these water-filled channels, we suggest a simple Hamiltonian model for the free energy profile of the molecule-pore interaction. The diffusional flux of molecules through channels is then calculated with the analytic solution to the Nernst-Planck equation, provided the chemical potential difference at the sides of the membrane is known. Being based on the clear physical conception, the parameters of the model may be obtained from the all-atom MD simulations for a membrane channel and the molecules separately. Eventually, enhanced sampling techniques combined with all-atom MD simulations allow testing the channel-molecule interaction model. Further, the model may be considered as a scoring function for fast quantification of the pore permeability for molecules with the parameters fit to the available experimental data. This, in particular, opens up the possibility for the computational screening of virtual libraries of possible modifications of an antibiotic in order to improve its permeability through the membrane.

*Speaker

Materials Science

Study of the ferroelectric properties of epitaxially strained SrTaO2N by means of DFT all-electrons first principles calculations.

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Recently, ferroelectric behavior was observed in compressively strained SrTaO2N thin films epitaxially grown on SrTiO3 substrates. Piezoresponse force microscopy measurements revealed small domains (101 –102 nm) that exhibited classical ferroelectricity, a behavior not previously observed in perovskite oxynitrides. The surrounding matrix region exhibited relaxor ferroelectric-like behavior, with remanent polarization invoked by domain poling. Bulk SrTaO2N samples do not show ferroelectricity, thus suggesting that the origin of it may be related with the strain induced by the substrate. Previous first-principles calculations suggested that the small domains and the surrounding matrix had trans-type and a cis-type anion arrangements, respectively, but do not address for the experimentally observed equilibrium phase, nor the strain dependent polarization. In this work, we present for the first time high accurate all-electron first-principles calculations on the different possible local structures that can explain the ferroelectric-like and relaxor properties of the strained material. The local structure and oxygen/nitrogen ordering has been related with polarization and epitaxial strain. We present the potential energies and polarization as functions of the in-plane lattice constant.

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Interplay between morphology and properties of core-shell Fe@Au nanoparticles

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Magnetic metallic nanoparticles (NPs) provide promising applications, especially in biomedicine. The NPs properties can be tuned by controlling the NPs size, shape and composition. For biomedical applications, the problem of the NP oxidation can be overcome by passivating the surface with a bio-compatible metal such as gold. Experimentalists from CEMES (Toulouse) have managed to grow highly facetted Fe@Au core-shell NPs of _˜8-10 nm using vapor phase deposition techniques [1]. These NPs display an original polyhedral core–shell morphology in which a Fe nanocube core acts as a nanosubstrate for the epitaxial growth of gold islands with a truncated pyramid shape. Interestingly, pure Fe NPs grown in the same conditions mostly exhibit a rounded shape, and the cubic morphology only appears after Au coverage.
In this work, we present a multi-scale computational modeling of these objects with the aim of understanding the key parameters that control their morphology and their properties. Structural and electronic properties of the interface between the core and the shell and of the NP surface have been investigated by DFT as a function of the shell thickness [2,3,4]. From these results, we built a Fe-Au interaction potential of the EAM type [5], which is used to study the evolution of the NP morphology as a function of size and Fe/Au volume ratio.

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*Speaker

Keynote: Car and Parrinello meet Green and Kubo: simulating heat transport from ab initio equilibrium molecular dynamics.

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Modern simulation methods based on electronic-structure theory have long been deemed unfit to compute heat transport coefficients within the Green-Kubo formalism. This is so because the quantum-mechanical energy density from which the heat flux is derived is inherently ill defined, thus allegedly hampering the use of the Green-Kubo formula. While this objection would actually apply to classical systems as well, I will demonstrate that the thermal conductivity is indeed independent of the specific microscopic expression for the energy density and current from which it is derived. This independence results from a kind of *gauge invariance* stemming from energy conservation and extensivity, which I will illustrate numerically for a classical Lennard-Jones fluid. I will then introduce an expression for the adiabatic energy flux, derived within density-functional theory, that allows simulating atomic heat transport using equilibrium *ab initio molecular dynamics*. The resulting methodology is demonstrated by comparing results from ab-initio and classical molecular-dynamics simulations of a model liquid-Argon system, for which accurate inter-atomic potentials are derived by the force-matching method, and applied to compute the thermal conductivity of heavy water at ambient conditions. The problem of evaluating transport coefficients along with their accuracy from relatively short trajectories is finally addressed and discussed with a few representative examples.

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Embedded many-body perturbation theories for organic optoelectronics

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Organic systems, for applications in photovoltaics, light-emitting devices, or photo-catalysis, stand as a challenge to ab initio simulations due to their disordered nature that complicates the standard periodic boundary treatment popular for inorganic semiconductors. In this presenta- tion, we will overview the use of many-body perturbation theories (MBPT), namely the GW and Bethe-Salpeter equation (BSE) formalisms, to explore the electronic and optical proper- ties of molecular systems. [1,2] Beyond gas phase calculations, we shown that "embedding" or "QM/MM" techniques, combining MBPT with continuous or discrete polarisable models, allow to describe dense organic systems, fully accounting for the electrostatic and dielectric environ- ment. [3] As a first application, we will show that the development of such techniques allows to unravel the mechanisms at stake in the molecular doping of organic semiconductors, [4] a crucial issue that remains much less understood than the standard doping in inorganic semiconductors.

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Optical properties of single-molecule junctions

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The Metal/Molecule/Metal nanojunctions are powerful devices for investigating phenomena involved in the domain of molecular electronics. Nowadays, thanks to the scanning tunneling microscope, it is possible to assemble atoms and molecules for building molecular junctions, to measure and manipulate their electric properties at the nanometric scale[1], and to excite these devices to induce optical transitions from one state to another[2]. In addition, molecular junctions are suitable systems for theoretical investigations with ab initio methods, since both size (few thousands atoms) and characteristic timescale of optical phenomena occurring (picoseconds) are accessible to the current high performance computing systems, allowing for a direct comparison to experiment.
In this talk, I will present density functional theory (DFT) and time-dependent DFT results concerning a single-molecule light-emitting diode, composed of a thiophene- and porphyrine-based molecule grafted between two gold electrodes, a device recently developed in our laboratory [2,3]. The electric current crossing the nanodiode acts as a local source for molecular excitations. We will focus on the emission spectra of such a device, paying particular attention to the vibronic transitions occurring in the nanojunction.

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*Speaker

Absence of spin edge polarization of acenes in the long-chain limit

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Spin polarized edges of graphene nanoribbons in the zig-zag configuration have been predicted by DFT calculations [1]. Only recently, graphene nanoribbons have been synthesized with zigzag edge topology [2]. Measurements revealed the presence of edge states that, if spin polarized, would be appealing for possible spintronic based applications. By accurate quantum Monte Carlo calculations, we show that the acenes, which can be seen as graphene nanoribbons with single unit width, do not possess spin polarized edge states. We reveal the key role played by electronic correlations to destroys the stability of the corresponding open shell-singlet state.

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Chemisorption of Hydroxides on Carbon and Boron Nitride Nanomaterials from Ab Initio Calculations.

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Recent nanofluidic experiments revealed strongly different surface charge measurements for boron-nitride (BN) and carbon nanotubes when in contact with saline and alkaline water. These observations contrast with the similar reactivity of a graphene layer and its BN counterpart, using density functional theory (DFT) framework, for intact and dissociative adsorption of gaseous water molecules. We investigate, by DFT in implicit water, single and multiple adsorption of anionic hydroxide on single layers. A differential adsorption strength is found in vacuum for the first ionic adsorption on the two materials - chemisorbed on BN while physisorbed on graphene. The effect of implicit solvation reduces all adsorption values, resulting in a favorable (nonfavorable) adsorption on BN (graphene). We also calculate a pKa=6 for BN in water, in good agreement with experiments. Comparatively, the unfavorable results for graphene in water echo the weaker surface charge measurements but point to an alternative scenario.
Various carbon and boron nitride allotropes are currently tested to probe possible effects of stacking, chirality and curvature. The adsorption of alternative ions are also investigated to determine the charging mechanism of the carbon surface.

*Speaker

On screening in organic semi conductors

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The weak screening in organic semiconductors is largely responsible for the low efficiency of organic bulk hetero junction solar cells [1] and strategies have been proposed to modify organic semiconductors to enhance their screening [2]. To contribute to this effort, we developed a method [3] for predicting the screening in organic semi conductors in their bulk phases from first principles. Here we describe our technique and the results of first tests on typical materials. The application of our method to new hypothetical organic semi conductors will require collaboration with synthetic chemists.

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*Speaker

Development of a joint refinement model for the one-electron reduced density matrix using different data sets

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Quantum mechanics teaches us that a many-body system is completely characterized by the wavefunction. However, in general, we are not interested in complete wavefunction but rather in the expectation value of some physical observables. The reduced density-matrix functional theory is a promissing alternative approach to describe a system of N particles [1,2]. This approach guarantees that the expectation value of any physical observable of a system in its ground state is a unique functional of the ground state one-electron reduced density matrix (1RDM).
Up to now, several models have been proposed to refine only the diagonal elements of 1RDM with a good accuracy, such as Hansen & Coppens multipolar model [3] or spin split model [4]. However, in this work, we have developed a model which allows to reconstruct all the elements of the 1RDM using simultaneously different data sets (magnetic structure factors and Compton profiles). Our implementation for a finite system is based on an expansion of the natural orbitals on Gaussian basis sets.

In this conference, we will first explain the main ingredients of our model. Then, we will present the first results of our algorithm, focussing on the calculation of the 1RDM, spin density, residual density, Bader analysis, and the Compton profiles. We will show that our model give very satisfactory results compared to the experimental data.

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*Speaker

Quantum effect on site preference and diffusion of interstitial hydrogen in face-centered cubic metals

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Measuring the rate of diffusion of hydrogen (H) in metals is important for understanding the kinetics of H storage and H-induced deterioration of materials. However, a consensus on the physical mechanisms and numerical values of H diffusivity for metals is still lacking. In this study, we investigated the site preference and diffusion behavior of interstitial H in several face-centered cubic (fcc) metals, such as Pd, Al, and Cu, by performing path-integral molecular dynamics (PIMD) modeling in the framework of density functional theory (DFT). This was necessary as the H atom has sufficiently low mass that it exhibits significant nuclear quantum delocalization and zero-point motion even at ambient temperature. First, the minimum energy path (MEP) and the transition state of H migration along the path between the octahedral (O) and the tetrahedral (T) interstitial sites were obtained using the climbing image nudged elastic band method based on DFT for a Pd32H and Al32H supercell. The DFT results showed that the H-migration barriers (Em) in Pd and Al exhibited similar values (approximately 0.16 eV), while the H atoms were stable at O sites for Pd and at T sites for Al. Then, the quantum effects on the activation free energies for H migration were characterized according to the PIMD-based free-energy profile obtained from the thermodynamic integration of the centroid force along the MEP at 150-600 K. We confirmed that the quantum effects significantly affected the Em and the difference between the energies of the H atom at the O site and the T site (Eo-t); The Em and Eo-t values in Pd at 300 K increased by 32% and 98%, respectively, relative to the classical limit. In contrast, the Em and Eo-t values in Al at 300 K decreased by 3% and 41%, respectively. This suggested that the quantum nature of H nuclei was essential for understanding the H-diffusion kinetics in these metals even at ambient temperature. It is noted that the apparent activation energies of 0.23 eV and 0.15 eV for Pd and Al, respectively, derived from the PIMD results were in good agreement with those from the experiments. The approach was found to provide a good description of the H-diffusion behaviors in Pd and Al over a wide temperature range.

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Multiscale Modeling of the Insertion and Diffusion of H-3 and Cl-36 in UNGG Graphite

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In order to optimize the waste management of nuclear graphite used in power plants, it is important to understand the properties of the activated impurities it contains, such as tritium and chlorine-36. A multiscale approach was therefore applied in order to study the local interaction of the radionuclides with the graphite matrix as well as diffusion and trapping mechanisms that occur on the nm-μm length scale. First, we studied the interaction of tritium and chlorine-36 with defects in graphite with density functional theory (DFT). While the bonding of hydrogen is mostly covalent for chemisorption and van der Waals for physisorption, the behavior of chlorine is much more complex. Depending on the defect site, both, dominantly covalent and dominantly charge transfer bonding, is observed. Following that, we used ab initio results to create a bond order potential to model the interaction of chlorine and the graphite matrix, which attributes for both, short and long range interactions. For the tritium-graphite interactions, the bond order potential AIREBO/M was used. These potentials were combined with the bond order potential LCBOP, which describes the C-C interactions. Since irradiated nuclear graphite is a complex system with crystalline, amorphous as well as porous zones, several different model structures were created to account for this diversity. The insertion and diffusion in these model structures was then studied for both radionuclides to evaluate the temperature dependence of these properties.

*Speaker

Numerical analysis of Brillouin zone integration methods

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I will introduce a numerical analysis of methods for the integration of quantities in the Brillouin zone. This yields rigorous error bounds, allowing for the selection of numerical parameters and guiding the development of more advanced methods. Joint work with E. Cancès, V. Ehrlacher, D. Gontier and D. Lombardi.

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On the oxidation state of titanium in titanium dioxide

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The oxidation state of titanium in titanium dioxide is commonly assumed to be +4. This assumption is used ubiquitously to rationalize phenomena observed with this widely used and technologically important material, although there does not seem to be a direct and independent experimental evidence to support this claim. Furthermore, recent theoretical investigations regularly indicated a charge remainder on Ti in titania compounds.
We present a comprehensive, theoretical and computational electronic structure investigation of Ti ions, titanium dioxide molecules, and titania bulk crystals which suggests a lower oxidation state. We analyzed charge density distributions in these systems qualitatively and quantitatively based on results of density functional theory and wave function-based calculations.

We conclude that there is evidence of a significant remaining contribution from valence *s* and *d* electrons of Ti, including the presence of a nuclear cusp around the Ti core. The charge corresponding to valence *s* and *d* states of Ti amounts to 1 *e*. The commonly assumed picture may therefore have to be revised.

*Speaker

Molecular dynamics modeling of graphite and graphene melting

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Experimental data on the melting line of graphite and thermodynamic properties of liquid carbon still remain controversial despite the long history of investigation [1]. The results of several dozen experimental works cover the wide span from 3800 to 5000 K for the graphite melting temperature Tm that is an essentially larger uncertainty than the errors of individual experiments. In this talk, extending our results [2] based on molecular dynamics (MD) and several accurate interatomic potential for carbon, we report our new results on the kinetics of graphite melting and aspects of defect formation in superheated single graphene layer. We determine by thermodynamic integration a relatively low value of Tm $\approx$ 3650 K for graphite. Our results suggest that at the heating rates higher that 10^6 K/s graphite specimens in most cases become superheated and the solid-liquid transition temperature becomes higher than the equilibrium melting temperature (up to 500-1000 K above Tm). The slow melting kinetics of graphite observed in our calculations and its high stability in the superheated state allows us to give a quantitative explanation of the long-standing discrepancy in the experimental data on Tm. Additionally, comparing melting kinetics for AIREBO potential and several REAX-FF parametrizations for carbon, we discuss the influence of the MD interatomic model and torsion-angle terms on the phase transition parameters.

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*Speaker

Ab initio study of inorganic perovskites: towards the prediction of PbZr_1-x_Ti_x_O_3 (PZT) IR spectrum

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Physical and chemical properties of materials are dependent on its chemical composition, its thickness, the temperature,... New applications of materials can be developed if we understand the link between these factors, their fabrication conditions and their phase transitions. PbZr1-xTixO3 (PZT), for instance, is commonly used for its high piezoelectric effect at x=0.48 (morphotropic, tetragonal / rhombohedral, phase boundary) but is currently studied for its possible interest in the information storage (RAM). To do so, the AILES beamline team of SOLEIL chose IR spectroscopy [Ref. 1].

However, to fully interpret the experimental spectra, theoretical modelling is necessary [Ref. 2]. In order to model PZT, the first step was to correctly reproduce the previous experimental and theoretical results on PbTiO3 (PT) and PbZrO3 (PZ) with a same set of parameters. In this purpose, we used the Density Functional Theory (DFT) code CRYSTAL 2014 which allows the application of the Linear Combination of Atomic Orbitals (LCAO) method on periodic systems. Structure geometry optimisations and electronic structure calculations were performed first. Then, harmonic vibrational frequencies were determined for transverse optical (TO) phonons, as well as those for longitudinal optical (LO) phonons, by way of the density functional perturbative theory (DFPT). Comparison with previous experimental and theoretical results permitted to find a set of parameters well suited to correctly describe both PT, PZ and, hopefully, PZT.

Next step is the study of PZT. We started with the case x=0.75. As it is a solid solution we cannot define a unique lattice. Thus it was decided to use the supercell (2'2'2) technique and to consider the 5 independent configurations (*i.e.* the different ways to distribute Ti and Zr atoms inside the supercell). Each configuration has a different space group (Pm, Pmm2, Cm11, P1 and Cm11) that seem incompatible with the tetragonal geometry observed experimentally. However, our geometry optimisation results show a good accordance with the experimental ones. Indeed, even though none of these configurations is of tetragonal space group, they have their geometrical characteristics (lattice parameters and $\alpha=\beta=\gamma=90\circ$) with a small difference between the lattice parameters of each configuration. Moreover, the IR absorption spectrum of one of the configurations has been calculated and compared to the simulated spectra of PT and PZ (Figure 1). As we can see, PZT IR spectrum

*Speaker

is similar to the PT one, with the appearance of some PZ features, confirmed by the comparison of wavevectors associated to the phonon modes.

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Buckled monolayer of GaAs under transverse electric field

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Buckled GaAs monolayer has a direct band gap semiconductor with energy gap of 1.31 eV in the absent of electric field. When we applied transverse electric field, the value of band gap decreases with increasing of electric field strength. In our previous work, it is observed that the buckled GaAs monolayer becomes metallic at 1.3 V/Å. In present work, we investigate the optical properties such as photon energy-dependent dielectric functions, extinction coefficient, refractive index, absorption spectrum and reflectivity of buckled GaAs monolayer in the semiconducting phase i.e. absence of external electric field and metallic phase i.e. presence of external electric field using density function theory.

*Speaker

Accurate ground-state correlation energies within the RPA and beyond: Theory and applications to molecules and zeolites

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Despite the high computational cost the adiabatic connection fluctuation dissipation theorem (ACFDT) represents a promising approach to improve the description of the electronic correlation within density functional theory. The simplest approximation that can be applied in the context of the ACFDT is the random phase approximation (RPA). We first show that the RPA can be efficiently computed within a plane-wave implementation by using dielectric eigenpotentials as a compact auxiliary basis set and the Lanczos algorithm. Then, we demonstrate that the accuracy of the RPA can be significantly improved by introducing a kernel containing an approximate electron-hole exchange term. This kernel leads to two beyond-RPA methods: An adiabatic connection analog of the second order screened exchange (AC-SOSEX) and an approximate electron-hole time-dependent Hartree-Fock (eh-TDHF). A series of applications to molecules and solids are presented to demonstrate the efficiency and accuracy of these methods. Importantly, it will be shown that the highly accurate beyond-RPA methods can be scaled to treat molecular systems with one hundred electrons requiring a basis set with hundreds of thousands of plane-waves. The ACFDT methods are then used to compute finite-temperature adsorption energies in zeolites by sampling multiple configurations generated by a molecular-dynamics simulation. This work was supported by Agence Nationale de la Recherche under grant number ANR-15-CE29-0003-01.

*Speaker

Atomistic Simulations of the Assembly of Large Gold Nanocrystals

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The assembly of gold nanocrystals coated with alkanethiolates are studied by Molecular Dynamics simulations. Body-centered cubic and face-centered cubic assemblies are compared. Due to the use of massively parallel computations, the assembly of nanocrystals up to 5 nm has been modelled with high precision [1,2], while previous simulations were restricted to 3 nm. This enables us to calculate accurate distances between the nanocrystals and compare them with models and experiments. Actually, two different models were proposed in the literature to calculate these distances [3,4]. We show that only the OCM (overlapping cone model) yields correct predictions in good agreement with the atomistic simulations and experiments. A detailed analysis is given to explain the success of the OCM model.

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*Speaker

UV-Visible Absorption Spectra of Silver Clusters from TDDFT Calculations.

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The absorption spectra of silver nanoparticles are characterized by a strong response in the UV-visible range, usually interpreted in the framework of (semi-)classical optics in terms of plasmon excitations due to the s electrons (Mie's Theory). Recently, Time-Dependent Density-Functional Theory (TDDFT) calculations have been shown to well reproduce the experimental spectra of metal nanoclusters when using range-separated hybrid (RSH) functionals. This approach gives a new description of the plasmon phenomenon from a quantum point of view. It also gives a framework to investigate the optical properties of small-sized metal clusters for which the classical approaches are no longer valid.

*Speaker

Unraveling the Icosahedral geometry of a light lanthanoid ion in a protic ionic liquid: a combined Molecular Dynamics and EXAFS study.

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Solvation is a complex phenomenon at the basis of the chemical behavior and reaction processes in liquids. The solvation properties of a particular class of metal ions, lanthanoid(III) ions Ln(III), in solvents with different polarity are of special interest due to the huge number of possible applications, such as the separation of these species in several industrial and nuclear processes.[1] Among possible solvents, Ionic Liquids (ILs) may be particularly suitable due to their unique properties such as high thermal and chemical stability, non-volatility, non-flammability and favorable solvating ability. Understanding the coordination properties of Ln(III) ions in ILs is therefore important for the development of innovative and best performing solvents. Among ILs, ethylammonium nitrate (EAN) belongs to the protic class, meaning that it is formed by proton transfer from a Bronsted acid to a Bronsted base, and it is the earliest reported example of a room-temperature IL.[2]
Here, a diluted solution of Ce(III) nitrate in EAN is investigated using molecular dynamics (MD) simulations and extended X-ray absorption fine structure (EXAFS) spectroscopy. This integrated MD-EXAFS strategy is a powerful approach to investigate disordered systems,[3,4] giving the possibility to obtain a reliable and conclusive determination of the coordination geometries of ions in liquid systems.

From a theoretical point of view, for the first time polarization is included in the MD force field to describe the coordination properties of a heavy metal ion in a protic IL. An innovative tool to predict the geometry of the polyhedra present in solution has also been developed, based on the combination of MD radial and angular distribution functions. We will show that the Ce(III) ion first solvation shell is formed by nitrate anions arranged in an icosahedral structure, with an equilbrium between monodentate and bidentate ligands existing in the solution, at variance with the typical tricapped trigonal prism (TTP) geometry that the Ce(III) ion forms in water.

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On the coordination of the Zn(II) ion in bistriflimide-based Ionic Liquids: Structural and dynamics properties at varying nature of the cation.

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Ionic Liquids (ILs) are interesting compounds that come with highly tunable properties and a low environmental impact, due to their thermal and chemical stability, as well as negligible vapor pressure and non-flammability. ILs have been employed in many applications as solvents, of which an interesting one is Zn deposition for Zn-air batteries.[1,2] Although a wide array of studies have been reported on the subject, information on the solvation properties of Zn salts in ILs and how those properties are influenced by the choice of the IL cation and anion are still lacking. This is due to the difficulty of obtaining reliable structural data and identify species in IL solutions.
In this work, a combination of X-ray absorption spectroscopy (XAS) and molecular dynamics (MD) has been employed to study four solutions of zinc bis(trifluoromethanesulfonyl)imide (Zn(Tf2N)2) in Tf2N based ILs in order to shed light on the influence that the IL organic cation has on the structural properties of Zn-Tf2N solvation complexes. This combination has been already proven a valuable approach for the study of IL solutions: the high selectivity and versatility of the XAS technique allows one to obtain reliable data on liquid samples, while MD simulations provide a dynamic atomistic description of the systems.[3,4]

We show that varying the IL cation has no influence on the close range arrangement of atoms around the Zn(II) cation up to 3.5 Å, with the metal ion coordinated in a typical octahedral site. Conversely, the choice of the organic cation has a significant impact on the speciation of the metal ion and on the dynamic properties of the Zn-Tf2N solvation complexes.

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Electronic and Structural Properties of K-doped NiO Mott-Insulator : Quantum Monte Carlo Study

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Doped Mott-insulators are of particular interest in thin film magnetic heterostructures and high temperature superconductivity. NiO systems have attracted a great deal of attention as a prototypical Mott-insulator and their electronic properties have been intensively studied theoretically using first-principle calculations. However, due to the strong contribution of the electronic correlations in transition metal oxides these systems are famously difficult to describe with methods such as density functional theory (DFT). Therefore, the accurate description of NiO properties and the prediction of its electronic properties in presence of defects is a challenging tasks using first principle calculations. Quantum Monte Carlo (QMC) is a many-body quantum theory solving explicitly the electronic correlations with a limited number of controlled approximations. In this study, we investigate the electronic and structural properties of K-doped AFM-II type bulk NiO system using QMC. Our results are then compared to various DFT approximations including correlation corrected schemes (such as DFT+U).

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*Speaker

Quantum model of optical properties and thermal emission of superradiant electronic excitations

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Light-matter interaction, usually considered only as a weak probe, becomes the dominant energy relaxation mechanism for collective excitations in a two-dimensional electron gas. Indeed, when the concentration is sufficiently high, electrons respond to the solicitation of photons as a whole, with an absorption spectrum presenting a single resonance at a completely different energy with respect to that of the electronic transitions [1]. This optical resonance corresponds to a many-body excitation of the system that ties together all dipoles, thus presenting a huge interaction with light. The spontaneous emission rate becomes proportional to the number of particles taking part in the collective excitation, a phenomenon known as superradiance [2]. In systems with very high electronic density, spontaneous emission is therefore the dominant relaxation mechanism and the associated broadening can even become a sizable fraction of the resonance frequency [3].
In this work we present a quantum model of optical properties and thermal emission of superradiant electronic excitations, the multisubband plasmons [4, 5, 6]. Our model relies on quantum Langevin equations, describing the dynamics of multisubband plasmons, coupled with an electronic and a photonic bath, which account for both radiative and non-radiative damping of the collective electronic excitations. We use input-output formalism [7] to solve the non-Markovian equations for the dynamics of the coupled system. For an optical input, we calculate the optical properties of the electron gas. We demonstrate that, when the radiative broadening, due to superradiance, becomes comparable to the energy of the plasmon, light-matter interaction becomes a non-perturbative phenomenon. This physical situation is correctly described only by taking into account the anti-resonant terms of the light-matter interaction Hamiltonian similarly to the ultra-strong coupling regime in micro-cavities. We have also applied our formalism to the case of an electronic input, showing that Kirchhoff's law of thermal emission is a consequence of our general assumptions [4,5].

When a stack of several quantum wells along the growth direction is considered, we show that plasmons localized in different regions of space exchange real and virtual photons. They thus behave as a collection of macro-atoms located on different positions along the growth direction. The exchange of real photons among the different plasmons gives rise to Dicke superradiance, resulting

*Speaker

in an increased spontaneous emission rate. Absorption and re-emission of virtual photons, triggered by vacuum fluctuations, result in a Lamb shift of the plasmon energy. Our theoretical results are in excellent agreement with experimental observations [6].

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Phonon-phonon interactions in semiconductors and in bismuth, and their effect on the electronic and thermal transport.

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Many semiconducting or bismuth-based materials are used in applications for the conversion of the energy, for instance in photovoltaic or thermoelectric devices. Understanding the electronic and thermal transport in these materials and nanostructures requires to be able to predict the electron-phonon [1,2] and phonon-phonon scattering processes [3], and to couple them with transport equations. In present work, electron-phonon and phonon-phonon interactions have been computed at the level of linear response within the density functional perturbation theory, and linearized Boltzmann Transport Equations (BTEs) have been used for the electron and phonon systems [4,5]. Moreover, for the study of thermoelectricity, we have combined BTEs for electrons and phonons and computed the effect of electron-phonon interaction, known as the phonon-drag contribution to the Seebeck coefficient.
As a highlight for the case of phonon-phonon interaction, and the effect of nanostructuring on this interaction, we will take the example of the thermal transport in bulk bismuth and in Bi-nanostructures. [6,7,8]. We will also show the influence of the nanostructure size and shape on the phonon-drag contribution of the thermoelectric coefficient of silicon [8].

This work has been done in collaboration with Lorenzo Paulatto, Michele Lazzeri, from IMPMC [Université Pierre et Marie Curie, CNRS 4 place Jussieu, F-75005 Paris, France], and with Francesco Mauri, [Dipartimento di Fisica, Universit'a di Roma La Sapienza, Piazzale Aldo Moro 5, I-00185 Roma, Italy]. We acknowledge support from the LABEX PALM (project Femtonic), the French DGA, and from the Chaire Énergie of the École Polytechnique. Results have been obtained with the Quantum ESPRESSO package. Computer time has been granted by GENCI (project 2210) and by Ecole Polytechnique through the LLR-LSI project.

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Regulation of structure and thermoelectric properties of the smallest SnTe nanowires via encapsulation within single-walled carbon nanotubes

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The properties and structure of a material may undergo dramatic change under confinement [1-3]. In cases when confinement is extreme, crystals can form quasi-one-dimensional (1D) structures that are often unstable otherwise. Single-walled carbon nanotubes (SWCNT) with diameters ranging from 8Å to 14 Å can be used as the confining environment for formation of such nano-wires from various compounds [4, 5]. The most stable stoichiometry, crystal structure and functional properties of a compound can differ significantly under confinement.

In this work we study 1D crystalline SnTe embedded in SWCNT and map the effect of varying degrees of confinement on the resulting nanowire and its thermoelectric properties. By adapting*ab initio* random structure searching, we discover several competitive structures of SnTe that can be formed within SWCNT and compare results with experimentally obtained encapsulated SnTe nanowires. We use a graphical representation of the Maxwell construction and the convex hull, which allows us to visualize the dependence of formation energy on stoichiometry. From first principles, we obtain the relative stability of the studied structures as a function of SWCNT diameter.

Finally, the discovered structures are studied with respect to their thermoelectric properties. We demonstrate a considerable effect of radius on the effective mass of charge carriers, and consequently, high electrical conductivity and thermopower. These findings establish a route for regulation of structure and thermoelectric properties via synthesis of SnTe extreme nanowires within appropriate SWCNT templates.

*Speaker

Multiscale modelling of nanoscale materials and electronic transport

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Simulation becomes increasingly important to understand phenomena at the nanoscale and develop novel materials. In recent years, we have developed multiscale simulation approaches for de-novo characterization and optimization of materials and device properties on the basis of their nanoscale constituents. Small-molecule organic semiconductors are used in a wide spectrum of applications, ranging from organic light emitting diodes to organic photovoltaics. However, the low carrier mobility severely limits their potential, e.g. for large area devices. As an example of our methodology, we present a parameter-free model1, which provides an accurate prediction of experimental data over ten orders of magnitude in mobility, and allows for the decomposition of the carrier mobility into molecule-specific quantities. We also demonstrate that a single molecular property, i.e. the dependence of the orbital energy on conformation, is the key factor defining mobility for hole transport materials2. The availability of first-principles models to compute key performance characteristics of organic semiconductors may enable in-silico screening of numerous chemical compounds for the development of highly efficient opto-electronic devices3, 4.

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Structural and dynamical properties of methane hydrate under high pressure via Raman spectroscopy and first-principles molecular dynamics including nuclear quantum effects.

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Methane hydrates (MH) are ice cages containing methane molecules. They can form spontaneously at the bottom of oceans and play a significant role in the formation of the outer planets of the solar system. Some phases, such as MH-III, have been shown to be stable for pressures exceeding 2 GPa, up to about 80 GPa [1]. The symmetrization of the H bonds under pressure in the ice skeleton has been postulated but not directly probed so far ; another issue concerns the interaction of the methane molecules with the ice network, as cages shrink under pressure.
We study MH-III in a wide pressure range, up to 65 GPa, by means of first-principles molecular dynamics. As nuclear quantum effects, mainly zero-point energy and tunneling, are relevant in the symmetrization of H bonds in ice [2,3], they are included by using the Quantum Thermal Bath (QTB) [4,5]. Systematic comparison between classical versus QTB simulations allows us to distinguish classical thermal effects from nuclear quantum effects on the MH-III properties.

In accordance with experimental results, we obtain a H bonds symmetrization transition, both thermally and quantum driven, as a function of pressure. We also provide a full description of structural and dynamical microscopic behaviors. In particular, strong coupling between the rotation of CH4 molecules and their distortions, as well as with the cage vibrational modes, are observed. Direct comparison with Raman data on samples that have been accurately synthesized is carried out through the analysis of time-dependent correlation functions.

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Energy Storage and Production

Proton Mobility in Protic Ionic Liquids: New Results from Theoretical Calculations.

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Ionic liquids (ILs) are salts made by bulky, sterically mismatched molecular ions that possess a low melting point owing to the fact that the electrostatic interactions are weakened and lattice formation frustrated by geometric effects. In contrast to traditional organic solvents, ILs possess negligible flammability and volatility and represent a new class of "green" solvents that are inherently safer than conventional solvents. A Protic Ionic Liquid (PIL) is formed through an acid base reaction. When the difference of pKa between the acid and the conjugate acid of the base is large ($>$ 10 pKa units) the ensuing liquid is completely ionized. In this case, the acidic proton is transferred quantitatively from the acid to the base during the synthesis reaction and turns out to be strongly bound to the latter. Subsequent proton transfer is therefore not possible. Conduction in these liquids is therefore due to ion drift (Walden mechanism) and inversely proportional to the liquid viscosity. In order to have a larger conductivity one has to find a way to promote the formation of different charge carriers. One possibility is to have proton transfer from one molecular ion to another. Compounds where amino acids in their deprotonated (anionic) form are combined with inorganic cations such as [Ch][Asp] and [Ch][Cys] might have these features. The former has a weak acid terminal, while the latter has a weak basic proton attached to the sulphur atom. We will show evidences of a non-ordinary behavior of these two materials that have been obtained by carefully validated ab-initio and classical molecular dynamics simulations.

*Speaker

Keynote: Understanding Ionic liquids role in energy application from calculations

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Ionic liquids (ILs) possess a wide range of properties and one of the only properties that can be thought of as ubiquitous among ILs is ion conductivity making them a promising material class for energy application.[1] Utilizing state of the art theoretical methods, [2] helps in understanding these liquids on the atomic level.
By examining their fundamental interactions,[3] the solvents' nanostructure,[4] the behaviour of ions with respect to ion pairing [5] and the complex behaviour with different materials, we gained molecular level insight into these liquids. Although this insight seems to be far away from comprehending a full device, it nevertheless helped us understanding the ILs' behaviour in such devices.

In a further step we studied significant effects with respect to gas absorption [6], we explored ILs as potential electrolytes for dye sensitized solar cells [7] and we considered their application for batteries. [8]

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Confinement Effects on an Electron Transfer Reaction in Nanoporous Carbon Electrodes

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Nanoconfinement effects strongly impact on many liquid properties, such as transport, diffusion coefficients, phase transitions, and solvation structures.[1,2] They are particularly important for supercapacitors, which have emerged as a complimentary energy stroage solution to batteries.[3] The effects has been observed to have a significant influence on the performance of supercapacitors, as has been demonstrated by experiment[4] and simulation[5], where it was shown that the use of materials with sub nanometric pores as electrodes greatly increase the capacitance of these devices. Within the realm of electrochemical applications, room temperature ionic liquids (RTILs) have attracted a considerable attention. Here we investigate how the electrochemical reactivity in such media may be impacted inside nanoporous carbon electrodes. We perform a molecular dynamics study of Fe3+/Fe2+ electron transfer (ET) reaction. The redox couple is dissolved in the 1-ethyl-3 methylimidazolium tetrafluoroborate (EMIM-BF4) RTIL, which is put in contact with carbide-derived carbon (CDC) nanoporous electrodes. The electrodes are held at constant electric potential by allowing the atomic charges on the carbon atoms to fluctuate. From the theoretical point of view, ET reactions in solution are usually studied in the framework of Marcus theory, which aims at accounting for the influence of solvent fluctuations on the rate of ET.[6] We show that the Fe3+/Fe2+ couple dissolved in EMIM-BF4 exhibits a deviation with respect to the standard Marcus theory. This behavior is rationalized by the stabilization of a solvation state of the Fe3+ cation in the disordered nanoporous electrode that is not observed in the bulk. The Fe3+ cation, which is tetracoordinated in the bulk, admits two stable solvation states in the nanoporous material: tetracoordinated and hexacoordinated. To account for this deviation we use the two-Gaussian solvation model,[7] from which the free energy curves for all the redox species in their various solvation states were extracted. This allows us to qualitatively analyze the effect of the confinement on the ET reaction. The fluctuations in the structure of the solvation shell of Fe3+ are shown to have a negligible effect from a thermodynamic point of view. In addition, it is shown that the activation energy of the associated ET process is much higher for the hexacoordinated form. It is therefore likely that the stabilization of this solvation state will result in a slow down of the ET reaction kinetic. This work is a first step

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towards a deeper understanding of the influence of the confinement on the ET in redox supercapacitor devices, which will be extended in the future to promising systems such as biredox RTILs.[8] The techniques developed in this work could also provide useful information for the development of ionic liquids-based thermo-electrochemical cells.

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Comparative Density Functional Theory - Density Functional Tight Binding study of fullerene derivatives: effects of addends, buckyball size, and crystallinity on properties affecting solar cell functionality

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Fullerene derivatives are the most widely used acceptor material in organic solar cells and as ETL in OPV-type perovskite cells.[1] While C60-PCBM has been the most popular choice, other molecules, either C70-based or using different addents, have led to better performance depending on the donor used and type of cell.[2] It is difficult to disambiguate effects due to molecular choice from other factors affecting experiments. For rational rather than ad hoc design, it is therefore important to have a theoretical/computational comparison of different fullerene derivatives which would identify the effects of various addents on key properties affecting solar cell performance such as the reduction potential, reorganization energy, etc.
While there exist computational studies picking up the "low hanging fruit" by standard DFT calculations on selected fullerenes as free molecules[3], the effects of the fullerene choice on the oxidation potential, electron and hole transport and optical properties remain largely unstudied. This has to do with significant effects due to aggregate state e.g. crystallinity on these properties, which are costlier to compute ab initio[4].

We present a comparative density functional based computational study of a dozen popular fullerene derivatives differing by the type of fullerene (C60 or C70) as well as by type and number of addends. We not only compare the electronic and optical properties of single molecules but also *account for the effects of crystallinity*, including effects on band structure (redox potentials) as well as calculations of electron and hole transfer rates between molecular units in a given crystal structure. To optimize crystal structure, Density Functional Tight Binding is used. We find that it is possible to modulate the band edges by about 0.5 eV by the choice of fullerene derivative. The electron and hole transfer rate change by 2 orders of magnitude depending on the molecule and direction and are computed to be in the range 10^9...12 s^-1.

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MODELLING NANOPOROUS GRAPHENE-BASED SUPERCAPACITORS

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Humanity is demanding a larger amount of energy as its level of development increases, due to which energy storage is one of the most important technologies nowadays. In this context, supercapacitors are currently considered as one of the most promising energy store devices [1], not only due to their higher energy density compared to conventional capacitors, but also because they exhibit better power performance than batteries. However, they are still not able to store the same amount of energy as the latter, so their capacitance performance needs to be optimized in order to be used in a greater number of applications. Many research efforts have been recently made to achieve this purpose while maintaining their high power capability and their long cycling life, either by using novel electrode materials with increased capacitance or by means of new electrolytes with wider potential windows such as ionic liquids [2]. The use of carbon-based materials as electrodes in supercapacitors has increased due to their relatively low cost and good properties, as well as the very good performance they have shown up to now [3]. Similarly, ionic liquids, whose key advantages are related to their unique properties and their tunable behavior, might play a fundamental role in the development of high energy and safer supercapacitors [4].
In this work, we have carried out a series of molecular dynamics simulations of a common ionic liquid confined between nanoporous graphene-based electrodes with the aim of gaining insight into the ion local structure under confinement. The ionic liquid was represented by a coarse-grained model, and the electrodes were maintained at constant potential by allowing the charge of the carbons of the electrode (represented by Gaussian distribution centered on the atom) to fluctuate at each time step of the simulation, which is of fundamental importance to obtain a realistic behavior of the electrolyte/electrode interface [5]. We present a comparison between the capacitance and the liquid structure in systems with different types of electrodes: carbide-derived carbon, graphite and perforated graphene sheets [6,7].

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Geosciences and Climate Modeling

Hierarchies of complexity in Earth System Modeling

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In "On Exactitude in Science", the Argentinian writer Borges tells the parable of a nation bankrupted by its cartographers, who endeavoured to create a map of the country on the scale of the country itself. It is sometimes argued that builders of Earth System models, which continue to grow in resolution and complexity, somewhat resemble Borges' mapmakers. Models so intricate that their behaviour is as rich and mysterious as the planet's itself, may not advance the science of climate as much as we would like.

In an influential essay, Isaac Held indicated how we may bridge this "gap between simulation and understanding". We construct *hierarchies of models*, with a range of complexity: simpler ones that embody a particular mechanism that underlies some aspect of the full Earth system, to comprehensive general circulation models with an interactive carbon cycle. An impressive range of models form the toolkit of Earth System Science: simplified forms of the primitive equations to study rotating fluids, largey eddy simulat (LES) models to study turbulence, cloud-resolving models, and so on, up to comprehensive Earth System Models (ESMs). Similarly there are modeling experiments also forming a hierarchy from highly idealized settings to the attempts to recreate the observed climate history in all its glory.

A key challenge is how to make the hierarchy more effective, so that we may readily isolate observed behaviour of a complex model in a simpler one, and represent findings from idealized models in GCMs. We present an overview of results from a recent workshop held in Princeton, NJ (https://www.wcrp-climate.org/gc-model-hierarchies-home), showing how the model hierarchy is deepening understanding of many mechanisms underlying the complex workings of the Earth System.

*Speaker

Importance of a fully anharmonic treatment of equilibrium isotope fractionation properties of dissolved ionic species as evidenced by Li+(aq)

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Equilibrium fractionation of stable isotopes is critically important in fields ranging from chemistry, including medicinal chemistry, electrochemistry, geochemistry, and nuclear chemistry, to environmental science. The dearth of reliable estimates of equilibrium fractionation factors, from experiment or from natural observations, creates a need for accurate computational approaches. Because isotope fractionation is a purely quantum mechanical phenomenon, exact calculation of fractionation factors is nontrivial. Consequently, a severe approximation is often made, in which it is assumed that the system can be decomposed into a set of independent harmonic oscillators.
A class of problems for which one might expect the harmonic approximation to perform most poorly is the isotopic fractionation between solid and solution phases.

In order to illustrate the errors associated with the harmonic approximation, we have considered the fractionation of Li isotopes between aqueous solution and phyllosilicate minerals, where we find that the harmonic approximation overestimates isotope fractionation factors by 30% at 25∘C.
Moving beyond the harmonic approximation requires tackling the problem of performing exact quantum calculations, which can be performed using the Feynman path integral formulation of quantum statistical mechanics. In the path integral approach, a system of quantum particles is represented as a set of classical-like ring-polymer chains, whose interparticle interactions are determined by the rules of quantum mechanics. Because a classical isomorphism exists between the true quantum system and the system of ring-polymers, classical-like methods can be applied.
Recent developments of efficient path integral approaches for the exact calculation of isotope fractionation now allow the case of the aforementioned dissolved Li fractionation properties to be studied in detail.
We find that the calculations yield results that are in good agreement with both experimental data and natural observations. Importantly, path integral methods, being fully atomistic, allow us to

*Speaker

identify the origins of anharmonic effects and to make reliable predictions at temperatures that are experimentally inaccessible yet are, nevertheless, relevant for natural phenomena.

Bridging the Scale Hierarchy Problem in Biogeochemical Models

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Ocean biogeochemical models are expressed in terms of coupled advection-reaction-diffusion equations. Numerical difficulties arise because the Péclet numbers in the ocean are enormous, therefore the scalar fields have structure at scales so small that they cannot possibly be resolved with today's supercomputers (nor tomorrow's...).
In numerical schemes based on fixed (Eulerian) grids the concentrations at a node represent locally averaged quantities. In a more or less explicit way, all these schemes describe the fluxes associated with unresolved small-scale processes by means of some sort of diffusion operator. This is acceptable in the absence of nonlinear reaction kinetics, when the unresolved scalar fluctuations play no large-scale dynamical role. In their presence, this approach leads to questionable results, because the nonlinear reaction terms generally don't commute with averaging operators. We show with simple test cases that this non-commutativity in practice means that large-scale features of the solution of the equations may be dramatically affected by the intensity of the scalar fluxes associated with the unresolved small scale processes.

In the absence of diffusion, the problem of unresolved structures would be easily overcome by using a Lagrangian framework, in place of an Eulerian one. Through the method of characteristics, an advection-reaction problem can be turned into a set of ODEs, for which many fast and accurate numerical integrators are available. Each ODE can be seen as describing processes occurring on an individual fluid particle as it is advected by the flow. Even when the number of particles is too small to properly resolve all the structures generated by the dynamics, the values of the scalar fields at the position of the particles are pointwise samples, and do not represent spatial averages. Thus the reaction terms are left unbiased.

For oceanographical applications the purely lagrangian scheme is insufficient: small scale processes do induce diffusion-like fluxes, and these, albeit tiny, are not negligible. Thus we propose to augment the simple Lagrangian method mentioned above with diffusive couplers among nearby fluid particles which mimic the fluxes due to the unresolved small-scale processes. The strength of these couplers is tunable, recovering the purely Lagrangian method in the limit of zero diffusivity, and is completely independent of the resolution. Therefore, the fluxes that affect the reaction terms are solely a modeling choice, and are not required for maintaining the stability (or other good properties) of the numerical scheme.
We present a number of test cases in which the Lagrangian methods plus a diffusive coupler is compared to known analytic results. We then compare our method with conventional numerical

*Speaker

simulations on Eulerian grids, showing the superiority of the first when the fine structures of the solution are not resolved.

Investigating the properties of silicate and carbonate melts at Earth's mantle conditions by molecular dynamics simulation

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Most of the Earth's mantle (between 35 and 2900 km depth) is made up of solid silicate rocks. However the dynamics of Earth's interior and the resulting volcanism (including plate tectonics) are essentially ruled by silicate melts, though they represent a very small fraction of the mantle (only 1% in mass). Among others, melt density and viscosity are key properties, since they rule the melt dynamics in the mantle and the eruptive style when it reaches the surface. Furthermore, carbon in the mantle is mainly stored as carbonates which can initiate a partial melting of the silicate matrix. The resulting carbonatitic melt could be the origin of highly electrically conductive zones probed in the upper mantle. Classical molecular dynamics is a powerful tool to investigate the physical properties of silicate and carbonate melts at both high temperature and high pressure that prevail in the mantle. We have recently developed empirical force fields for natural silicate melts and molten carbonates of various compositions. The thermodynamic properties (EOS, density...) and the transport coefficients (viscosity, electrical conductivity...) can be calculated with an insight into the atomic structure, providing valuable information on the melts at the Earth's mantle conditions.

*Speaker

Keynote: Towards high-resolution climate models

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Climate change is a pressing societal challenge and a difficult and fascinating scientific topic. Current climate projections are largely based on global climate models (GCMs) with horizontal resolutions around 100 km. Despite much progress, the uncertainty of climate projections has hardly narrowed in the last two decades. In order to better represent the multi-scale interactions in the climate system, comprehensive efforts are underway to refine the horizontal resolution of global and regional climate models to O(1 km), with the intent to represent deep clouds explicitly, rather than using semi-empirical parameterizations. This refinement would move climate models closer to first principles, and is expected to reduce the uncertainties of climate projections. High resolution is particularly attractive in order to better represent critical cloud feedback processes as well as the water cycle, including the simulation of extreme events (such as heavy precipitation events and floods). The presentation will be illustrated with decade-long simulations at km-scale horizontal resolution covering the European continent (Leutwyler et al. 2016, GMD; Leutwyler et al. 2017, JGR, in press). A discussion will be provided of key challenges affecting the numerical and computational design of future high-resolution climate models. It is argued that already today, modern supercomputers would in principle enable global atmospheric kilometer-scale climate simulations, provided appropriately refactored codes were available, and provided appropriate solutions were found to cope with the rapidly growing output volumes.

*Speaker

Education

Groundstates of liquid crystals with colloids: a project for undergraduate students.

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Although simulated annealing has become a useful tool for optimization of many systems, its initial raison d'etre of achieving the groundstate structure for a spin or atomic/molecular condensed system remains important. Such modelling, whether by analog models such as glass beads or by simple computer models can be suited to undergraduate projects. In this presentation we discuss the application of simulated annealing to find the groundstate of a system of liquid crystals with suspended colloids. These are expected to have interesting conductive behaviour, relevant to applications for television and computer screens. In our first stage, a pure liquid crystal system was simulated and vizualized by undergraduates and presented on an educational website. In this next stage colloid(s) were added, and the original code modified accordingly. Interesting effects such as ordering around the colloid have been seen and will be described. Comments on using bead systems to assist students in understanding these processes will also be made.

*Speaker

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Toolkit-based approach to undergraduate training in molecular dynamics

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There is a high starting inertia in computation for many reasons. Molecular dynamics computation is not exempt. What is apparent is that unlike empirically based research, breaking into computation can require a monumental effort. This paper is aimed at offsetting these requirements using an approach based on locally developed toolkit for molecular dynamics running on a standalone computer. The specific objectives are to facilitate the review of techniques through a rational derivation of concise mathematical models and algorithms that are quickly testable and accurate for a well-defined class problems, given the wealth of published literature results for comparison. In taking this approach, we develop a toolkit of reusable MD functions in the C/C++ language in a compact, library repository that work on both Linux and Windows. The approach is proving to be popular with our higher level undergraduates interested in computation.

*Speaker

Time evolution of the unstable soliton solution for dust acoustic waves with trapped electrons

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The positive dust charged grains is considered as the immobile particles compared to ions and electrons.
Some electrons can be trapped in the dust charge potential while some move freely in the plasma. The reductive perturbation method shows that the weakly nonlinear waves equation gives a soliton solution. The spectral method is applied for the time evolution of the perturbed soliton solution to the sinusoidal funtion with the longwavelength.
The higher soliton can be found for the unstable soliton.

*Speaker

Posters

P1: Propagation of Dust-Ion Acoustic (DIA) waves in multi-species plasma with Cairn's distributed electrons, quantum effects in inertia less electrons and ions

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Dust Ion Acoustic Waves (DIAW) are studied in this multispecies plasma consisting of negatively charged dusts, Cairn's di stributed electrons, cold ions and inertia less electrons with quantum effects. Interesting characteristics of DIAWs are investigated by employing pseudopotential method deriving the corr esponding energy integral. Compressive, rarefactive and only subsonic solitons are shown to exist in this investigation. For different values of the Mach number, the model is found to generate small amplitude subsonic compressive and rarefactive solitons. These small amplitude solitons are very sensitive to the non thermal parameter β occurring in the Cairn's distributed electrons. This β plays an important role throughout the investigation and remarkably β is directly proportional to the amplitudes of the DIA solitons. Also, the number of dust charges (Z_d) contained in dust particles are found to influence the growth of DIA subsonic solitons. The quantum effect in electrons perceptibly takes the role of the formation of solitary waves in this multi component plasma.

*Speaker

P2: Investigation of dust ion acoustic (DIA) solitons in multicomponent plasma with relativistic ions and Cairns distributed electrons

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The effect of relativistic ions supplemented by Cairns distributed electrons is introduced to establish solitary waves in multicomponent plasma. The dependence of DIA solitons on the non-thermal parameter β reflexes a new light in this investigation. The simultaneous existence of both compressive and rarefective relativistic solitons earmarking a critical region of non-existence of KdV solitons is an interesting feature of this investigation. Besides in the right part of the asymptotic line through critical Z_{dc} separating into two disjoint existence regions exhibits growth of solitons from compressive to rarefective solitons as Z_d increases but in the left part of it, there exists only rarefective relativistic solitons for all $\sigma = 0.02$, 0.03 and 0.04 and for fixed values of the parameters $\alpha = 0.1$, $\beta = 0.7$, $u_{i0} = 0.1$, $u_{d0} = 0.2$ and $c = 300$. The existence of high amplitude rarefective solitons is shown to diminish with the non-thermal parameter β for all $Z_d = 30$, 60, 90 and for fixed values of the other parameters of the system. The upper limit of this non thermal parameter $\beta < 1$ for nonexistence of rarefective solitons is a new feature of this pursuit. Also the relativistic only compressive solitons are established for higher value of $\beta = 1$ (exceeding the upper limit) which slowly increase with $u_{d0} < 8$ within the small range of $Z_d = 10$,20,30 and for fixed values of the other parameters. But they are shown to first increase concavely after a critical value of u_{dc} near it.

*Speaker

P3: The role of the order of perturbation and its determination in the process of enforcing discrete Korteweg-de-Vries solitons to modified Korte-de-Vries solitons as means of continuum hypothesis in a multi component dusty plasma'

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In general,the motion of fluids,so also plasmas is considered under continuum hypothesis as continous system within certain mathematical limitation though actually it is discrete.This idea can rightly be represented for example in investigating modified Korteweg-de-Vries(mKdV) solitons in plasmas from the transformed discrete KdV solitons.On the basis of the standard transformation of the stretched variables ,the KdV equation is derived to study solitary waves in plasma.But setting the non linear coefficient p=0,the system is turned into discrete and employing higher order perturbation in the stretching cordinates,the mKdV equation is derived which admits soliton solution in plasma.To speak the truth,a discrete system is transformed into a continous system under continuum hypothesis.But the role of the order of perturbation and determination of its magnitudes are nowhere discussed till now. In this endevour,it is tried to explore various orders of perturbation to generate solitary waves of respective amplitudes through mKdV equation in multi component plasma consisting of Cairns distributed electrons,another component of electrons with quantum effects,stationary dusts and the usual ions.Remarkable feature in this pursuit is to determine amplitudes of mKdV solitons corresponding to each order of perturbation(Eepsilon)ion streaming vio, non thermal parameter 'beta' and the number of dust charge Zd. This is the first approach in this direction.

*Speaker

P4: Complexity Cmp and Time's Arrow

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Cmp, as a measure of short time series complexity, defined recently using permutation and linear combination. Time's arrow is related here to the increasing of complexity Cmp. Three origins of time's arrow are considered. The first origin is interaction of a quantum system with the environment, where we prefer the Mensky's interpretation of quantum mechanics. The second one is the reaching of equilibrium state of an isolated thermodynamic system, equalizing temperature, pressure and molecule concentration (increasing of entropy). The third origin of time's arrow is the accelerated expansion of the Universe. A planet orbits a star which rest frame S' is approximately inertial, in a short time. Using Lorenz velocity transformation, we compute complexity of this motion in the observer rest inertial frame S. Cmp is increasing if the velocity of S' frame relative to S frame is increasing.

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P5: Computational studying energy and spectral parameters of hadronic (pionic) atoms with account of the strong pion-nuclear interaction

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We present an effective relativistic computational approach to studying the energy and spectral characteristics of hadronic (pionic) atoms based on the Klein-Gordon-Fock equation with optimized p–N interaction optical potential and relativistic many-body perturbation theory with Dirac-Breit-Kohn-Sham zeroth approximation Hamiltonian and correct treating radiation, electron-screening, nuclear effects (finite size, quadrupole deformation) effects [1,2]. It is developed a precise theory for calculating energy levels shifts and widths, provided by a strong p–N interaction ("strong" width) and the interaction of the pion with QED vacuum (radiation width) within the model optimized optical complex p–N interaction potential and relativistic energy approach based on the Gell-Mann and Low formalism with complex relativistic e-e interaction potential. For a number of heavy atoms, including, p– 165Ho,169Tm, 173Yb, 175Lu, 181Ta, 197Au, 203Tl, 208Pb, 209Bi, there are obtained the values 4f and 3d levels shifts and widths, caused by a strong p–N interaction, including correction directly related to the effect of nuclear quadrupole deformation. It has been carried out computing energy (electromagnetic) contributions (Coulomb, radiation corrections, incl. polarization of vacuum, such as Uehling-Serber, Wichman-Kroll and Kallen-Sabry ones, Breit-Rosenthal-Crawford-Schawlow effect etc.). It is shown that the electromagnetic corrections to the transition energies, in particular due to radiation effect, are up to _˜ 5 keV, nuclear ones - up to _˜ 0.2 keV and correction for electronic shielding due to the presence of the survived 2[He], 4 [Be], [Ne] electron shells is _˜ 0.07keV.

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P6: Computational studying the hyperfine and electroweak interaction and parity violation in heavy finite Fermi-systems: Advanced Code

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Now days the parity non-conservation effect in heavy atomic, nuclear and molecular systems has a potential to probe a new physics beyond the Standard Model. In our paper we systematically develop and apply new computational code to precise studying a parity violation effect in heavy atoms with account for the relativistic, nuclear and radiation QED corrections. Our approach is based on the formalism of the nuclear-QED many-body perturbation theory [1-3]. The nuclear block of theory is presented by the relativistic mean field model (the Dirac-Woods-Saxon model). As a test, we present the results of computing the energy levels, hyperfine structure intervals, E1,M1 radiation transitions amplitudes in the heavy atoms such as 133Cs, 173Yb, 205Tl. Further we have computed the parity violation radiative amplitudes for a number of the atomic and nuclear systems, namely: 133Cs, 173Yb, 205Tl (atomic parity violation) and 119,121Sn (nuclear parity violation). Accuracy of accounting for the inter electron exchange-correlation corrections, the Breit and weak e-e interactions, radiation & nuclear (magnetic moment distribution, finite size, neutron "skin") effects, nuclear spin dependent corrections due to an anapole moment, Z-boson [(AnVe) current] exchange, the hyperfine-Z boson exchange [(VnAe) current] have been analysed. Besides, the weak charge has been calculated for the 133Cs, 205Tl atoms and firstly 173Yb and comparison of the theoretical results with the Standard Model data has been done. Using the experimental parity non-conservation parameter value E/b=39mV/cm (Berkeley 2009; Tsigutkin et al) and our value 9.707×10**(-10)ea, it is easily to determine the weak charge value Qw=-92.31 for 173Yb (Z=70, N=103) that should be compared with the Standard Model value Qw=-95.44.
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*Speaker

P7: Confinement and Chiral Phase Transition in Dual QCD Formulation.

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Quark confinement and dynamical chiral-symmetry breaking are the most important non-perturbative phenomena in quantum chromodynamics (QCD). Within the context of this theory, the dual QCD formulation based on magnetic symmetry has been analyzed and its resulting flux tube structure has been investigated for analyzing the non-perturbative features of QCD. We investigate the dynamical chiral-symmetry breaking using Schwinger-Dyson equation, where the gluon propagator include non-perturbative effect related to color confinement. A close relation among the color confinement and chiral-symmetry breaking has been observed and demonstrated by computing the various dynamical parameters like quark mass, pion decay constant and the quark condensate characterizing the dynamical chiral symmetry breaking. The recovery of the chiral symmetry has also been discussed at finite temperature and a strong correlation between the critical temperature Tc of the chiral symmetry restoration and the strength of string tension has been observed.

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P8: SU(3) Dual QCD formulation and quark-hadron phase transition

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Based on the well known topological properties of non-abelian gauge theories, a dual QCD gauge theory is constructed in terms of magnetic symmetry, which manifest the topological structure of the symmetry group in a non-trivial way. The topological magnetic charges associated with monopoles have been brought into the dynamics by the possible homotopy $\Pi 2$ [SU (3)/U (1) $\otimes$ U (1)]. The dynamical breaking of the magnetic symmetry has been shown to impart the dual superconducting properties to the magnetically condensed QCD vacuum which ultimately leads to a unique flux tube configuration in QCD vacuum responsible for enforcing the color confinement. The color singlet physical spectrum in accordance with the color confinement has been achieved through the requirement of the color reflection invariance which provides two magnetic glueballs as the collective excitations of the magnetically condensed dual superconducting QCD vacuum which in turn, are intimately connected to the flux confining parameters (penetration length and coherence length) of the superconducting vacuum. Analyzing such dual version of QCD in thermal domain by constructing the hadronic bag using the confining part of the flux tube energy in dual QCD formulation, the thermodynamical description of hadron to Quark-Gluon Plasma (QGP) phase transition has been analyzed to study the various thermodynamical, bulk and transport properties of QGP. The various properties investigated are shown to provide the firm evidence of the first order phase transition and a mixed phase consisting of the QGP and the hadron phases. In order to investigate the dynamics of first order phase transition the associated surface tension of the mixed phase has also been investigated which is in remarkable agreement with lattice QCD finding and MIT bag model calculations. The physical picture for such phase transition has been shown to lead to a rapid increase in the degrees of freedom carried by quark and gluons and which have a deep relevance with the modern high energy experiments at the Relativistic Heavy Ion Collider (RHIC, BNL) and the Large Hadron Collider (LHC, CERN) with the possibility to explore the new high-energy form of matter(QGP) consisting of interacting quarks and gluons.

*Speaker

P9: Implications of general lepton mass matrices in the standard model for Neutrinoless Double Beta Decay parameter m_ee

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Within the framework of the standard model (SM), using the facility of weak basis (WB) transformations, the general Dirac neutrino mass matrix and the charged lepton mass matrix can essentially be considered as texture two zero mass matrices. Using type I seesaw formula for Majorana neutrino mass matrix, our analysis yields lower bounds $m_ee \geq 0.001$ eV for normal mass ordering and $m_ee \geq 0.08$ eV for inverted mass ordering, the latter being tantalizingly close to the expected outcome of the ongoing experiments. Interestingly, for inverted mass ordering, mee is largely independent of variation of mass m3, whereas, for normal mass ordering with m1 in the range 0.0001 eV–0.01 eV, the bound on parameter mee gets further sharpened and one obtains mee within the band 0.014–0.042 eV. Further, noting that a particular set of texture four zero quark mass matrices has been shown to be a unique viable option for the description of quark mixing data, an analysis of similar mass matrices in the lepton sector has also been carried out to obtain bounds for the parameter mee with interesting consequences.

*Speaker

P10: Advanced computational approach to studying Rydberg and autoionization resonances in spectra of heavy lanthanides and actinides

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The paper is devoted to further development and application of the a relativistic many-body perturbation theory [1] with Dirac-Kohn-Sham (DKS) zeroth approximation combined with the generalized energy approach to studying the spectra and autoionization resonances spectra for heavy atoms, in particular, atoms of lanthanides and actinides (Eu, Tm, Yb, U) and search of the unusual futures in behaviour of the autoionization resonances in sufficiently weak dc electric field that can be detected by a laser spectroscopy methods. The wave function zeroth basis is found from the Dirac equation with a potential, which includes ab initio (the optimized DKS potential, the electric potential of a nucleus). The correlation corrections of the PT high orders are taken into account within the Green functions method (with using the Feynman diagram's technique). All correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction, mass operator iterations) are taken into account. To test a new approach we list the experimental (compilation) and theoretical data for energies (accounted from the ground state: 4f146*s*2 1S0) of some YbI singly excited states, namely, data, obtained on the basis of multiconfiguration Hartree-Fock (MCHF) method within the framework of Breit-Pauli (BP) relativistic corrections developed by Fischer (different sets of configurations considered in MCHF-BP calculation]); data, obtained on the basis of Cowan's relativistic Hartree-Fock method; data of analysis by Wyart-Camus; data by Ivanov et al obtained on the basis of the model many-body perturbation theory and energy approach (EA-MMBPT) [2-4]. A significant part of data for studied elements is received for the first time. Besides, we firstly present numerical data on energies and widths of some Rydberg autoionization resonances in atoms of lanthanides and actinides (Eu, Tm, Yb, U) and give physically reasonable explanation of unusual properties of these resonances for atoms in a free state and in external DC electric field.

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P11: Advanced computational approach to nonlinear dynamics of laser systems with elements of a chaos

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The work is devoted to carrying out new approaches to the universal quantum-dynamic and chaos-geometric modelling, analysis and prediction of a chaotic dynamics of nonlinear processes in atomic and molecular systems in intense electromagnetic fields and quantum-generator and laser systems. The latter include a single-modal laser with an absorbing cell, a fiber laser, a semiconductor laser coupled with feedback with delay, the system of semiconductor quantum generators, combined through a general cavity. The computing code includes a set of numerical quantum-dynamic models and such non-linear analysis methods as the correlation integral approach, multi-fractal analysis, average mutual information, surrogate data, false nearest neighbours algorithms, the Lyapunov's exponents and Kolmogorov entropy approach, spectral methods and nonlinear prediction (predicted trajectories, neural network etc) algorithms [1]. We present new approach to modelling a chaotic dynamics of atomic and molecular systems in a uniform magnetic and crossed magnetic and AC electric fields. It includes the combined finite-difference solution of the Schr´odinger equation, optimized operator perturbation theory, the model potential method for atomic systems in a field [2].
We present the results of the complete numerical investigation of a chaos generation in the low- and high-attractor time dynamics of the semiconductor GaAs/GaAlAs laser system with delayed feedback (the governing parameter: feedback strength or current injection). It has been numerically shown that firstly arising periodic states of the system transform into individual chaotic states and then global chaotic attractor with a chaos generation scenario through period-doubling bifurcation, which is significantly modified. We present firstly computed original data on the Lyapunov's exponents (+, +), correlation (chaos – 2.2; hyperchaos – 7.4), embedding (correspondingly 4 and 8), Kaplan-York (correspondingly 1.8 and 7.1) dimensions, the Kolmogorov entropy (0.15-0.71). Besides, It has been presented new model of forecasting the low-attractor time dynamics for the first time.

We present the results of the complete numerical investigation of a chaos generation in the low- and high-attractor time dynamics of the erbium one-ring fibre laser (EDFL, 20.9mV strength, l= 1550.190nm) with the control parameters: the modulation frequency f and dc bias voltage of the electro-optical modulator. It has been numerically shown that there are realized the one-period (f = 75MHz, V = 10V and f = 60MHz, V = 4V), two-period (f = 68 MHz, V = 10V or f = 60MHz, V = 6V) and chaotic (f = 64MHz, V = 10 V and f=60MHz, V=10V) dynamical regimes in dependence upon the *f, V* values. The Lyapunov's exponents (+, +), correlation, embedding, Kaplan-York dimensions, the Kolmogorov entropy have been computed. It has been numerically shown that a chaos

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in the EDFL is generated via intermittency by increasing the DC bias voltage and period-doubling bifurcation by reducing the frequency modulation computers.

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P12: Advanced relativistic model potential approach to computing the radiation transition characteristics for atoms and multicharged ions

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Accurate radiative decay widths and probabilities, oscillator strengths of atomic transitions are needed for example in astrophysics, thermonuclear plasma diagnostics, in fusion research and laser physics. Traditionally, advanced modeling is important and of current interest in the theory of atomic spectra and associated spectral lines. In our work we present an advanced relativistic model potential approach to compute radiation transition and ionization probabilities and oscillator strengths for alkali atoms and multicharhed ions. The starting master method includes the combined relativistic energy approach and relativistic many-body perturbation theory (PT) with the zeroth order, optimized one-particle approximation [1]. The key feature of the presented fundamental theory is an implementation of the relativistic model potential (one version) or quantum defect (second version) approximation into the framework of the S-matrix energy formalism, applicable to multi-electron atomic system. It provides sufficiently correct, and equally, simplified numerical procedure to evaluate the corresponding radiative transition and ionization properties. This approach appears significantly more advantageous when compared to the standard Hartree-Fock and Dirac-Fock methods. As illustration we computed energies and probabilities of the radiative transitions and ionization characteristics for Li-,Cs-, Fr-like multi-charged ions and neutral atoms. Our approach provides reasonable agreement with experiment. We evaluated that all results for oscillator strengths, obtained within our approach in different photon propagator gauges: G1-Coulomb, G2-Feynman; G3-Babushkin) are practically equal that is provided by using an effective QED energy procedure.

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P13: Advanced computational approach in electron-collisional spectroscopy of atoms and multicharged ions in plasmas

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A great number of physically different effects occur in atomic systems (ensembles) in dependence upon a intensity, frequency, multi-colority of laser field, energy spectrum structure of an atomic system etc. In the last decade a considerable interest has attracted studying of the elementary atomic processes in plasma environments because of the plasma screening effect on the plasma-embedded atomic systems. In this paper we present new advanced computational approach to electron-collisional spectroscopy of atoms and multicharged ions in plasmas, one-and two-color multi-photon spectroscopy of a number of transitions in a hydrogen, lithium and caesium atoms and ions (free and immersed in a Debye plasmas) is studied theoretically. The theoretical approach is based on the relativistic operator perturbation theory (PT) and relativistic energy approach [1]. The energy shift and width of the multiphoton resonances are calculated within an energy approach, which is based on the Gell-Mann and Low adiabatic formalism [2]. The plasmas medium effects are taken into account by introducing the Yukawa-type electron-nuclear attraction and electron-electron repulsion potentials into the electronic Hamiltonian for N-electron atom (ion) in a plasma [3]. There is studied a plasmas with typical corresponding parameters: the Debye lengths ID=5a.u. [solar core: temperature T=107K; density 10(32) m(-3)] and 25 a.u. [inertial confinement: temperature T=10(4)K; density 10(28) m(-3)] . It has been quantitatively determined a variation of the multi-photon resonance enhancement frequencies in dependence upon the plasmas parameters (the Debye length). For example, the corresponding values for the resonance enhancement frequencies $\omega r1$, $\omega r2$ and $\omega r3$ for the 1s–4f transition in the hydrogen for different Debye lengths (ID=5-50 a.u.) are between 0.009 and 0.023a.u. The H-plasma data are compared with available other data [2].

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P14: Cooperative laser electron-gamma-nuclear phenomena in dynamics and spectroscopy of molecules: Advanced Computational Code

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In the modern quantum optics and spectroscopy there is a new class of topics, connected with discovery and modelling the co-operative laser-electron-gamma-nuclear phenomena in the atoms, molecules and clusters. It includes a calculation of the probabilities and energies of the mixed g-optical quantum transitions in molecules (clusters), intensities of the complicated g-transitions due to the changing of the molecular excited states population under action of laser radiation, quantitative calculation of the "laser-electron-gamma-nuclear-molecule" systems [1,2]. The first qualitative estimates of the cooperative effects parameters were earlier presented (see [1] and refs. therein). Due to the emission or adsorption of the nuclear g-quantum in molecular system there is changing the electron vibration-rotation molecular states. We present an advanced computational approach to calculation of electron-nuclear g transition spectra (e-vibration satellites) of nucleus in a molecule (clusters), based on the relativistic density functional (DF) formalism and energy approach [3]. The relativistic effects are not very significant here, but such a formalism is important for proper treating multiple different decay channels. Decay and excitation probability are linked with imaginary part of the molecule - field system. New data on the electron-nuclear g-transition spectra of the nucleus in some multiatomics are presented for a number of molecules: 3-atomic XY2 (Dμh), 4-atomic XY3(D3h), 5-atomic XY4(Td), 7-atomic XY6(Oh) ones. As example, we present the results of computing emission and absorption spectrum of nucleus 127I in H127I and other diatomics. Besides, we list new data on probabilities of the first several vibrational-nuclear transitions in a case of the emission and absorption spectrum of nucleus 188Os (E(0)g= 155 keV) linked with molecule *OsO4*(recoil energy R= 0,051 eV).

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P15: New relativistic computational energy approach to heavy Fermi-systems in a super strong field: AC Stark and multi-photon resonances

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It is presented an advanced computational approach to studying interaction of the finite Fermi systems (heavy atoms, nuclei, molecules) with a strong external (DC electric and laser) field. It is based on the relativistic operator perturbation theory (PT), energy approach (Gell-Mann and Low adiabatic formalism) [1,2] and method of the relativistic Green's function for the Dirac equation with complex energy. Results of the computing the multi-photon resonance and ionization profile in Na,Cs, Ba atoms are listed [2]. We have studied the cases of single-, multi-mode, coherent, stochastic laser pulse shape. New data on the DC, AC strong field Stark resonances, multi-photon and autoionization resonances, ionization profiles for a few heavy atoms (Eu, Tm, Gd, U) are presented. It has been firstly studied a giant broadening effect of the autoionization resonance width in a sufficiently weak electric (laser) field for uranium It is declared that probably this effect is universal for optics and quantum chemistry of lanthanides and actinides and superheavy elements.
The direct interaction of super intense laser field (I_˜1025-1035 W/cm2) with nuclei is studied within the operator PT and the relativistic mean-field (plus Dirac-Woods-Saxon) model [2]. We present the results of computing AC Stark shifts of single proton states in the nuclei 16O, 168Er and compared these data with available data. New data are also listed for the 57Fe and 171Yb nuclei. Shifts of several keV are reached at intensities of roughly 10(34) W/cm(2) for 16O, 57Fe and 10(32) W/cm(2) for heavier nuclei. It is firstly presented a consistent relativistic theory of multiphoton-resonances in nuclei and first estimates of energies and widths for such resonances are presented for 57Fe and 171Yb nuclei

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P16: Advanced computational code to "shake-up" and NEET effects in laser electron-gamma-nuclear spectroscopy of atoms and ions

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A new class of problems has been arisen and connected with modelling the cooperative laser-electron-nuclear phenomena such as the electron shell shake-up and NEET or NEEC (nuclear excitation by electron transition or capture) effects in heavy neutral atomic/nuclear systems [1,2]. Though the shake-up effects in the neutral atoms (molecules) are quite weak (because of the weak coupling of the electron and nuclear degrees of freedom), the possibilities of their realization significantly change in a case of the multicharged ions. We present consistent, relativistic computational approach to calculation of the probabilities of the different cooperative laser electron-gamma-nuclear processes in the multicharged ions (including the characteristics of the electron satellites in gamma-spectra of nuclei of the multicharged ions and the resonant NEET (NEEC) effects in heavy nuclei of multicharged ion). The theory is based on the relativistic energy approach (S-matrix formalism of Gell-Mann and Low) [3,4] and relativistic many-body perturbation theory [5]. Within the energy approach, decay and excitation probability (of the electron shell shake-up process or etc) is linked with the imaginary part of energy of the excited state for the "electron shell-nucleus-photon" system. For radiative decays it is manifested as effect of retarding in interaction and self-action and calculated within QED perturbation theory formalism. We firstly present new data about intensities of the electron satellites in gamma-spectra of nuclei in the neutral (low lying transitions) and multicharged O-and F-like ions for isotopes Fe,Cs,Yb which demonstrate an existence of an new effect of the giant increasing (up 3 orders) electron satellites intensities (electron shell shake-up probabilities) under transition from the neutral atoms to the corresponding multicharged ions. We develop the similar relativistic energy approach to the NEET (NEEC) process in the heavy multicharged ions and present the advanced quantitative estimates of the corresponding NEET probabilities in the nuclei of Os,U, Au,Mt of the O-and F-like multicharged ions. The received data demonstrate an effect of the significant changing the corresponding NEET probabilities under transition from the neutral atomic/nuclear systems to the corresponding multicharged ions.

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P17: Modulation of Intense Femtosecond Laser Pulse by a strong magnetic field

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In this work, we investigate the modulated-polarization of an intense linearly polarized laser through an ionizing gaseous medium in the presence of an external strong magnetic field with arbitrary directions. Our simulation indicates that the laser polarization dramatically depends on the direction of the strong magnetic field. This striking phenomenon can be attributed to the collective movements of ionized electrons. Our above finding has implications in investigating the impact of self-generated strong magnetic field during the ultraintense laser-plasma interactions, and the generation of modulated-polarization light sources.

*Speaker

P18: Superexchange Interatomic Coulombic decay by Fano-ADC-Stieltjes method

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Fano-ADC-Stieltjes is an *ab initio L2* method for the decay width calculations of metastable states of atoms and molecules. It relies on Fano-Feshbach theory of resonances to describe bound-like discrete and continuum states and on algebraic diagrammatic construction in intermediate states representation (ISR-ADC) to construct many-electron wave functions. Correct renormalization of discretized continuum is achieved by Stieltjes imaging technique. Favorable numerical properties are fast convergence and size extensivity. We assess this method as the most efficient one for studying non-radiative relaxation processes such as Auger effect or Interatomic Coulombic decay (ICD). In ICD, an inner-valence vacancy is filled by an outer-valence electron and the excess energy is transferred to a neighboring atom which is thus ionized. We study new ICD mechanism called superexchange ICD in NeHeNe trimer. We demonstrate that the decay width of Ne dimer increases significantly in the presence of the bridge He atom. The enhancement is due to the electron transfer between the Ne atom and virtual states of the ICD-inactive He, driven by inter-atomic electron correlation.

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P19: PROJECTILE CHARGE EFFECT ON ELECTRON AND POSITRON IMPACT SINGLE IONIZATION CROSS SECTIONS OF PLASMA RELEVANT MOLECULAR TARGETS

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The charged particle impact ionization studies of fundamental atomic and molecular systems have been of great interest since the early days of quantum mechanics. Extensive theoretical and experimental investigations have been carried out to understand the electron and positron impact single ionization processes of various targets. [1-6]. Such type of studies are important in many areas, such as understanding the processes in the earth's upper atmosphere, in the development of new lasers and novel forms of lighting, as well as in the treatment of cancers that use radiotherapy. Triple differential cross section calculations for the ionization of 1e1,2a1 and 3a1,orbitals of the NH3 molecule by low energy electron, and positron impact are reported. The present investigation is done in the distorted wave born approximation (DWBA) using post collision interaction and polarization of target. We found a very good agreement with the experimental data of Nixon and Murray [7].

With changing the projectile's charge, significant differences were observed between the electron and positron impact ionization cross sections of NH3 molecules.

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P20: Computer simulation of the interaction of fullerene with nanographene

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Using energy minimization method the stable structures of both fullerene and defect-free nanographene were found. For description of the interatomic potential we used Brenner interatomic potential [1], which is specifically parameterized for the carbon systems. Then by the same energy minimization method and using the same Brenner potential, computer modeling of the interaction of fullerene with nanographene was carried out.
The results of computer simulations, the various structural changes of both fullerene and defect-free nanographene caused by their interaction as well as binding energies of these formed structures are presented and discussed.
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P21: Ab- initio calculation of the electronic gap, the refractif index of (PbTe), (SrTe) and Lead strontium telluride alloys (Pb1-xSrxTe).

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We have studied different physical properties of (PbTe), (SrTe), and (Pb1-*x*Sr*x*Te) semiconductors, using the *Ab-initio* full potential augmented plane wave (FP-LAPW) method. The two exchange potentials namely PBE-GGA and WC-GGA were considered, whilethe recentlydeveloped modified Becke and Johnson (mBJ) potential was employed to study theelectronic and optical properties. For these alloys, the band gaps as well as the lattice parameter increases with the amount of Sr while the bulk modulus and the refractive index decreases with the Sr concentration. We explained the microscopic origins of the band gap bowing, using the approach of Zenger and co-workers. At ambient conditions (P=0, T=0), we found that Pb1-xSrxTe is a direct band gap semiconductor R-R for x=0.25, 0.5 and 0.75. The refractive indices are also calculated using the (FP-LAPW) method and the models of Moss, Ravindra and the Erve-Vandame. The results obtained are compared with each other, for PbTe and SrTe show better agreement with the available data.
Keywords: DFT; Alloys; Electronic properties; Optical properties;

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P22: Quantum phase transition in a three-dimensional dimerized Heisenberg model on a corundum lattice

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We investigate a auantum phase transtion in a three-dimensional (3D) J-J' dimerized quantum Heisenberg model on a corundum lattice by exact diagonalization and quantum Monte Carlo simulations. We estimate the ctrictical point between spin single phase and magnetically orderd phase as (J'/J)_c = 0.36$. We also discuss the Z_2 topological number defined by the Berry phase for the spin singlet phase.

*Speaker

P23: Enhancement of superconducting correlations by charge and spin ordering in coupled electron and spin systems

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Projector Quantum-Monte-Carlo method is used to examine effects of the spin-independent U as well as spin-dependent J Coulomb interaction between the localized f and itinerant d electrons on the stability of various types of charge/spin ordering and superconducting correlations in the generalized spin-one-half Falicov-Kimball model with Hund and Hubbard coupling. The model is studied for a wide range of f and d-electron concentrations and it is found that the interband interactions U and J stabilize three basic types of charge/spin ordering, and namely, (i) the axial striped phases, (ii) the regular n-molecular phases and (iii) the phase separated states. It is shown that the d-wave pairing correlations are enhanced within the axial striped and phase separated states, but not in the regular phases. Moreover, it was found that the antiferromagnetic spin arrangement within the chains further enhances the d-wave paring correlations, while the ferromagnetic one has a fully opposite effect.

*Speaker

P24: Quantum Monte Carlo calculations of elastic properties of one-dimensional carbon chain

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Quantum Monte Carlo (QMC) calculations have been performed to estimate elastic properties of one-dimensional carbon chain, carbyne, which is the strongest material among carbon allotropes according to density functional theory (DFT) calculations [1]. Recent QMC study of carbon allotropes, however, revealed that the DFT-PBE calculations would overestimate their cohesive energies significantly [2], which is also confirmed by our present study on carbyne. We here compute the QMC total energies of carbyne under different strains to estimate its tensile stiffness and Young's modulus. The bending stiffness is also estimated from the QMC total energy of carbon ring as a function of the curvature. We report that the QMC tensile stiffness, bending stiffness, and Young's modulus of carbon chain are 33.0(2) eV/A^2, 2.41(1) eV.A, and 38.1(3) TPa, respectively, each of which is found be smaller than the corresponding DFT-PBE value by about 10 %. This leads us to conclude that the DFT-PBE overestimates not only the cohesive energy of carbyne but also its elastic properties.

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*Speaker

P25: Determination of energies dan wave functions of a quantum many-body system by the finite difference time domain (FDTD) with the Hartree Fock (HF) approximation

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The finite difference time domain (FDTD) method has been successfully applied to solve the time independent Schr´odinger equation for a one body quantum system. In this paper, we extend our FDTD method for a many body quantum system by using the Hartree-Fock (HF) approximation. The FDTD-HF method uses the time-dependent HF (TDHF) equation in imaginary time. The TDHF is numerically solved by the FDTD method with a constraint that single particle wave functions must be orthogonal in every iteration of the FDTD method. Numerical results for one, two and three dimensional systems are given and compared with the analytical results and the FDTD results without HF approximation. It is shown that the FDTD-HF method gives accurate results.

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P26: Prediction of electronic and optical properties of ZnAl2Te4 defect chalcopyrite semiconductor: an ab-initio study

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The defect chalcopyrite (DC) semiconductors are of greatest technological interest and have numerous applications in the fields of photovoltaic devices, photo detectors and nonlinear optics. Defect Chalcopyrite (DC) semiconductors with chemical formula AIIB2IIIC4VI are belongs to well-known family of AIBIIIC2VI ternary chalcopyrite semiconductors. The DC semiconductors are crystallized in tetragonal structure which is closely related to the chalcopyrite semiconductors, except former have stoichiometric vacancy in the positions of the cations. in the present study we have investigated the structural, electronic and optical properties of ZnAl2Te4 defect chalcopyrite semiconductor using generalized gradient approximation within density functional theory (DFT). We have calculated the optimized lattice constants (a and c) and comapred with the available experimental values. The optimized lattice consants have been used to calculate the energy gap and found to be 1.57 eV. The partial and total density of states have been discussed in detail. The frequency dependent dielectric consatnt and refractive index have been calculated and ploted in the energy range 0-13 eV. All the above parameters have been compared with the available experimental and theoritical values and found good agreement between them.

*Speaker

P27: Coarse analysis of non-equilibrium collective phenomena: Bifurcation analysis of the optimal velocity model using diffusion maps

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We present a general method to analyse macroscopic collective phenomena observed in non-equilibrium many-body systems.
For this purpose, we employ the method of diffusion maps, which is one of the dimensionality-reduction techniques. Using diffusion maps, we systematically define a few relevant coarse-grained variables to describe macroscopic phenomena. The time evolution of a macroscopic behaviour is described as a trajectory in the low-dimensional space constructed by these coarse variables. We apply this method to the analysis of the optimal velocity model and reveal a bifurcation structure, which features a transition to the emergence of a moving cluster, which is identified as traffic jam cluster. This property of the transition is observed in real highway traffic.

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P28: Monte Carlo Study of a Three States Spin Model

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We use the Monte Carlo simulation technique to study the critical behavior of a three-states spin model, with bilinear and biquadratic nearest-neighbor pair interactions in a square lattice, known as the Blume-Emery-Griffiths model(BEG).
In order to characterize this model, we study the phase diagram, in which we identify three different phases: Ferromagnetic, Paramagnetic and a Quadrupolar phase. Moreover, we study the behavior of the system by adding a next-nearest-neighbor interaction into the Quadrupolar phase.

We perform our studies by using two algorithms: Metropolis and Wang-Landau in the implementation proposed by Belardinelli-Pereyra, which not only estimates the density of states of the system, but also reduces the simulation time and the errors.

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P29: Study of the kinetic effects in homogeneous and heterogeneous bubble cavitation via atomistic simulations

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Cavitation is the formation of bubbles in the surrounding liquid. The formation of the liquid-vapor interface has an energetic cost which makes liquids very resilient to the growth of the new vapor/gas phase. However once formed and advected with the flow bubble give rise to extreme phenomena such as sonoluminescence [1], damage of pumps and turbines [2] and destruction of living tissues [3]. Controlling cavitation is therefore crucial in many scientific contexts. In particular, many fundamental aspect of the first stage of cavitation, the nucleation of bubbles, remain elusive and difficult to quantify.

Classical Nucleation Theory, which is based on simple continuum models, might fail to reproduce the actual nucleation rates. It is also very difficult to control the experimental conditions to tell whether cavitation is happening in homogeneous, i.e. in pure bulk liquid, or heterogeneous conditions, i.e. in presence of impurities that cataylize the process.

The nucleation event occurs on microscopic time and length scales, which makes atomistic models well suited to get insights in the phenomenon. In this work atomistic simulations are employed to study homogeneous and heterogeneous cavitation of metastable liquids at different thermodynamic conditions. Molecular dynamics is combined with Forward Flux Sampling technique [4] to evaluate the nucleation rates, allowing also the sampling of the ensemble of reactive paths. Performing a statistical analysis of the transition pathways, it is possible to assign a weight to the different reaction channels. This allows to identify which channels are kinetically preferred and which factors affect the inception of nucleation event.

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*Speaker

P30: The SAPBC method on local, non-cluster updates algorithms of Monte Carlo simulation: A study on more convergence of spin correlation at critical temperature.

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In this method, we propose computational technique of Screw-Antisymmetric Periodic Boundary Condition (**SAPBC Method**) on local, non-cluster update algorithms of Isotropic square lattice Ising model of Monte Carlo Simulations, as well. The **SAPBC Method**, actually, is an extended mixed method of Screw (helical) and Antisymmetric periodic boundary conditions beyond connection from of nearest neighbor spin of the main lattice to even far away block of the outer (foreign) neighbor spin arrays. Here, meanwhile of description of geometry exact details of method and way of spin interaction, have applied to critical slowing down in order to achieve more convergence of spin correlation at critical temperature. Actually, in general, at critical temperature algorithms performed by using **SAPBC Method** have faster correlation and much shorter autocorrelation time than algorithms performed by using PBC Method. We will also see that Autocorrelation function for the typewriter Metropolis algorithm was found to be zero at high temperatures. For low temperatures it fell to zero and stayed there. The **SAPBC Method** also confirms and consists with the law of the spatial correlation length with its dynamical critical exponent. Therefore, it can be used as a trenchant method applied to boundary conditions of Monte Carlo simulation problems extending on a variety of other models such as XY-Pots-Heisenberg model and also cluster algorithms such as Wolf, Swendsen-Wangas, Hoshen-Koppelman as well.

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P31: Fast customization of the Wang Landau parallel algorithm for the different lattices

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An efficient universal procedure was developed to construct a density of states from the data provided by the parallel implementation of the Wang Landau Monte Carlo based algorithm for the different spin lattices. The sampled energy space was shared between the individual threads with the controlled overlaps for the two-dimensional Ising and Pott models and their variants. The latest development of the algorithm in the form of the density of states replica exchange technique was considered. The several factors of immediate importance for the seamless stitching process have being implemented. Speed and universality of the parallel algorithm implementation as well as the data post-processing technique were combined to produce the expected smooth density of states.

*Speaker

P32: Mean squared displacement of dust particles in 2-dimensional strongly coupled Yukawa liquids exposed to an external magnetic field

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In various physical settings complex plasmas are affected by external electric and magnetic fields. In particular, the influence of magnetic fields on strongly coupled dusty plasmas became an important topic in the last few years [1,2].
The purpose of this work is to investigate the mean squared displacement of the dust particles exposed to a static homogeneous external magnetic field, under the effect of friction due to the presence of a neutral background gas. Computer simulations of the motion of the dust particles, interacting via a Yukawa potential (characterized by a screening parameter κ), have been carried out based on the Langevin equation of motion, which takes into account the influence of buffer gas/plasma environment on the dust particles' dynamics. The robust second-order Velocity-Verlet propagation scheme [3], obtained with taking into account an external magnetic field and background gas, was used in order to solve the equations of motion of the particles. The mean squared displacements of the particles were investigated in the wide region of the four dimensionless parameters: the coupling parameter, the screening parameter, the magnetic field strength expressed as the ratio of the cyclotron to plasma frequency, and the friction coefficient.

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*Speaker

P33: Multiple eigen-modes of Rayleigh-Taylor instability observed for a smoothly varying density fluid interface

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In this work, multiple eigen-systems including linear growth rates and eigen-functions have been discovered for the Rayleigh-Taylor instability by numerically solving the Sturm-Liouville eigen-value problem in the case of two-dimensional plane geometry. The system called the first mode has the maximal linear growth rate and is just extensively studied in literature. Higher modes have smaller eigen-values, but possess multi-peak eigen-functions which bring on multiple pairs of vortexes in the vorticity field. A general fitting expression for the first four eigen-modes is presented. Direct numerical simulations show that, the high modes lead to appearance of multilayered spike-bubble pairs, and lots of secondary spikes and bubbles are also generated due to the interactions between internal spikes and bubbles. The present work has potential applications in many research and engineering areas, e.g., in reducing the RTI growth during capsule implosions in inertial confinement fusion.

*Speaker

P34: Ion acoustic solitary waves with high relativistic thermal ions and non-thermal electrons and thermal positrons in plasma

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In this paper both compressive and rarefactive solitons are shown to exist in electron-positron-ion plasma consisting of high relativistic thermal ions, nonthermal electrons and thermal positrons. The compressive and rarefactive Korteweg-de Vries (KdV) solitons of small amplitude are shown to exist only for fast ion-acoustic mode. It has been found that the inclusion of variable temperature of the ion species not only significantly modifies the basic features of the ion-acoustic solitons but also introduces a new regime for the existence of solitons. Further, the increase in ion to electron temperature ratio results in decrease in soliton amplitude. Also it is found that increase in relativistic factor increases the soliton amplitude.

*Speaker

P35: Computational Model Of Calcium And IP3 Dynamics: A Finite Difference Method Approach

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Calcium signalling is one of the most important intracellular signalling mechanisms. A lot of approaches and investigators have been made on study of calcium signalling in various cells to understand its mechanisms over recent decades. However, most of existing investigators have mainly focussed on study of calcium signalling in various cells without paying attention to dependence of calcium signalling on other chemical ions like inositol-1; 4; 5 triphosphate ions etc. Some models for independent study of calcium signalling and inositol-1; 4; 5 triphosphate signalling in various cells are present but very little attention has been paid by the researchers to study the interdependence of these two signalling processes in a cell. In this paper, we propose a coupled mathematical model to understand the interdependence of inositol-1; 4; 5 triphosphate dynamics and calcium dynamics in a myocyte cell. Such studies will provide the deeper understanding of various factors involved in calcium signalling in myocytes, which may be of great use to biomedical scientists for various medical applications.
Keywords: calcium signalling; coupling; finite difference method; inositol-1; 4; 5 triphosphate

*Speaker

P36: DFT Computational and Spectroscopic Investigations on The Cyanide Bridged Heteronuclear Polymeric Complex: [Cd(N-Meim)2Ni(μ-CN)4]n

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The complex [Cd(N-meim)2Ni(μ-CN)4]n has been modelled in DFT/B3LYP and DFT/B3PW91 methods with using LANL2DZ basis set (Figure 1). The molecular structure and vibration spectral properties of the complex were insighted experimentally in the literature [1]. In this study, the molecular geometry was optimized on the basis of experimental geometry. Afterwards, vibration spectral properties were calculated using same quantum chemical methods and basis set. Then, fundamental vibrations were assigned on the basis of the potential energy distribution (PED). The FT-IR and Raman vibration modes were determined using both experimental and theoretical methods (Figure 2). According to the results, the good agreement was obtained between theoretical data and experimental ones. In this case, regression equations have been calculated, and these equations were obtained for B3LYP and B3PW91 calculations as y = 0.986x + 6.9431 R^2 = 0.9993; y = 0.9906x + 2.64 R^2 = 0.9993, respectively. Additionally, electronic transition energies (HOMO and LUMO energy levels) of the complex were calculated by time depended density functional theory with B3LYP and B3PW91 methods with LANL2DZ basis set. The transition energies between the HOMO and LUMO levels were determined as 0.727 eV for B3LYP and 0.736 eV for B3PW91 (Figure 3).
Keywords: Cyanide complex; Heteronuclear polymeric complex; DFT; B3LYP; B3PW91; HOMO-LUMO.

This study was supported financially by Eskişehir Osmangazi University Research Fund (Project No: BAP-201519047 (BAP 2015-830)).

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P37: High performance and low complexity algorithm for MP2 calculations in solids

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We present a low-complexity algorithm to calculate the correlation energy of periodic systems in second-order Moller-Plesset perturbation theory (MP2). In contrast to previous approximation-free MP2 codes, our implementation possesses a quartic scaling, O(N^4), with respect to the system size N and offers an almost ideal parallelization efficiency. The general issue that the correlation energy converges slowly with the number of basis functions is eased by an internal basis set extrapolation. The key concept to reduce the scaling is to eliminate all summations over virtual orbitals which can be elegantly achieved in the Laplace transformed MP2 (LTMP2) formulation using plane wave basis sets and Fast Fourier transforms. Analogously, this approach could allow to calculate second order screened exchange (SOSEX) as well as particle-hole ladder diagrams with a similar low complexity. Hence, the presented method can be considered as a step towards systematically improved correlation energies.

*Speaker

P38: Statistical vs non-statistical effects and the importance of the activation method in unimolecular fragmentation of peptides via chemical dynamics simulations

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Often a reliable description of the potential energy surface (PES) leads to a good knowledge and prevision of a reaction mechanism and the associated rate constants. However, non-statistical and non-equilibrium effects are often observed in reaction dynamics in both molecular dynamic simulations (MD) and experiments. Those influence the reactions in a way that their mechanisms and rate constants are not predictable by means of statistical theories as transition state theory, Rice-Ramsperger-Kassel-Marcus (RRKM).
Unimolecular dissociations should undergo into rapid and complete internal vibrational relaxation to be modelled through RRKM. However, this is not always observed, especially in gas phase where the system is not fast thermalized by the bath and fast processes are often favoured. The way in which the system is thermalized (or not) could, indeed, induce a statistical (or not) dissociation of the system. MD, where the electronic structure problem is solved *on-the-fly* and many trajectories are propagated provide useful information. Here we have studied gas phase reactivity using MD with semi-empirical Hamiltonians, which are compulsory when studying large systems.

We have recently studied the fragmentation different behaviour as obtained by direct dynamics simulations in which the system is vibrationally activated by explicit collisions and by a microcanonical energy activation for the deprotonated di-proline and doubly protonated peptides [1], TIK(H+)2 and TLK(H+)2[2,3]. Different pathways and mechanisms are observed depending on the activation way.

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Finally, we will explain in details the L-cysteine fragmentation, which appears experimentally different as function of the activation mode. The combination of collision simulations and PES study provided an explanation of such experimental observation.

P39: Fully quantum description of the Zundel ion: combining variational quantum Monte Carlo with path integral Langevin dynamics

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We develop a novel approach for a fully quantum description of coupled electron-ion systems from first principles. It combines the variational quantum Monte Carlo solution of the electronic part with the path integral formalism for the quantum nuclear dynamics. On the one hand, the path integral molecular dynamics includes nuclear quantum effects by adding a set of fictitious classical particles (beads) aimed at reproducing nuclear quantum fluctuations via a harmonic kinetic term. On the other hand, variational quantum Monte Carlo can provide Born-Oppenheimer potential energy surfaces with a precision comparable to the most advanced post Hartree-Fock approaches, and with a favorable scaling with the system size. In order to deal with the intrinsic noise due to the stochastic nature of quantum Monte Carlo methods, we generalize the path integral molecular dynamics using a Langevin thermostat correlated according to the covariance matrix of quantum Monte Carlo nuclear forces. The variational parameters of the quantum Monte Carlo wave function are evolved during the nuclear dynamics, such that the Born-Oppenheimer potential energy surface is unbiased. Statistical errors on the wave function parameters are reduced by resorting to bead grouping average, which we show to be accurate and well controlled. Our general algorithm relies on a Trotter breakup between the dynamics driven by ionic forces and the one set by the harmonic interbead couplings. The latter is exactly integrated even in presence of the Langevin thermostat, thanks to the mapping onto an Ornstein-Uhlenbeck process. This framework turns out to be very efficient also in the case of noiseless (deterministic) ionic forces. The new implementation is validated on the Zundel ion (H5O2+) by direct comparison with standard path integral Langevin dynamics calculations made with a coupled cluster potential energy surface. Nuclear quantum effects are confirmed to be dominant over thermal effects well beyond room temperature giving the excess proton an increased mobility by quantum tunneling.

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P40: Molecular, vibrational, electronic structure and nonlinear optical properties of 1-ethylimidazole

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In this study include quantum chemical calculations by combined most common spectroscopic techniques (FT-IR, Raman and UV-Vis spectra) for 1-ethylimidazole (etim). The following theoretical calculations are prepared by combined experimental results; firstly, geometry of the molecule are optimized by DFT/ B3LYP method with LANL2DZ, SDD and CEP-121G basis sets in the ground state and gas phase. The vibrational (FT-IR and Raman) spectra were investigated same method after optimization of the molecule and fundamental vibrational modes were assigned based on potential energy distributions (PED). Additionally, electronic transition energy was calculated with time depended density functional theory (TD-DFT) approach. HOMO and LUMO energies confirm that charge transfer occurs within the molecule. Molecular electro-static potential surface (MEPs) were also presented. Nonlinear optical properties (NLO) were given theoretically. The geometric parameters and normal vibration modes obtained from LANL2DZ calculations are in good agreement with the experimental data. An excellent correlation is seen between theoretical and experimental results. These results are provides a detailed description of the structural and a deep understanding of the characteristics physicochemical properties of the molecule.
Keywords: 1-Ethylimidazole; Structural and vibration analyses; Molecular electro-static potential surface (MEPs); Nonlinear optical properties (NLO).

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P41: Experimental and Computational Study on Photoreaction of Flutamide and Its Cyano Analogue

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Flutamide {2-methyl-*N*-[4-nitro-3-(trifluoromethyl)phenyl]- propanamide} and bicalutamide { *N*-[4-cyano-3-(trifluoromethyl)phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide} are a nonsteroidal antiandrogen drug that is widely used for the treatment of prostate cancer. It has been reported that photodermatosis is occasionally induced when an individual taking flutamide is exposed to sunlight. Compared to flutamide, there are few reports of photohypersensitivity with bicalutamide. In order to elucidate the reason why flutamide have caused photosensitivity, we investigate the photoreaction of flutamide and cyano analogue, which is the mimic of bicalutamide, experimentally and theoreticaly.

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P42: Application of order-N first-principles DFT calculations with temperature controlled molecular dynamics to biomolecular system

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Molecular simulation methodologies are now commonly used to explore biological phenomena of proteins and/or biomolecules. For example, molecular dynamics (MD) simulation methods are expected to help us understand the mechanism of time-dependent biological phenomena. Nowadays, quantum mechanics/molecular mechanics (QM/MM) hybrid methods and/or its molecular dynamics (QM/MM-MD) method are also used well in this field. Recently, we introduced stable MD method to the framework of our order-*N* first-principles density functional theory methodology. In this study, we demonstrate our order-*N* first-principles DFT calculations with temperature controlled molecular dynamics and investigate the short-time behavior for hydrated DNA system.

*Speaker

P43: A theoretical study on the molecular structure, vibrational (FT-IR and Raman) spectra and electronic transition energies of cyanide-bridged heteronuclear polymeric complex of 1-ethylimidazole: [Cu(etim)4Pd(μ-CN)4]n

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In this study, [Cu(etim)4Pd(μ-CN)4]n (etim=1-ethylimidazole) complex was constructed using the theoretical parameters determined from its structural, spectral and electric response properties using DFT with B3LYP and B3PW91 methods via LANL2DZ basis set in the ground state and gas phase (Figure 1). The geometrical parameters, vibrational wavenumbers and electronic transition energies were obtained; the fundamental vibrations were assigned on the basis of the potential energy distribution (PED). FT-IR and Raman vibration modes of the complex was determined using both experimental and theoretical methods (Figure 2). The theoretical vibration modes were scaled with 0.961 for the B3LYP method and 0.957 for the B3PW91 method. When the theoretical and experimental vibrational frequencies were examined, it was observed that the experimental vibration data above 1500 cm-1 is in agreement with the scaled theoretical vibration data for both methods. Similarly, the vibration frequencies below 1500 cm-1 are in good agreement with the unscaled theoretical vibration frequencies. Regression equations have been obtained in order to show the good agreement between the experimental and theoretical vibration modes. These equations were obtained for B3LYP and B3PW91 calculations as y = 0.9615x + 24.106 R^2 = 0.9961 and y = 0.9575x + 27.469; R^2 = 0.996, respectively. A good agreement was observed between obtained theoretical and experimental spectra in both methods. Additionally, non-linear optical properties such as the first order hyperpolarizability (β0) and other related properties (α0 and $\Delta\alpha$) were also computed. βo, α0 and $\Delta\alpha$ values were found as 9763x10-33 esu, 36.94x10-24 esu and 88.60x10-24 esu in B3PW91 method, respectively, whereas these values were obtained as 9733x10-33 esu, -37.31x10-24 esu and 89.61x10-24 esu in B3LYP method. The dipole moment and the first static hyperpolarization value of the urea molecule are used as reference for determining the nonlinear optical properties (β = 0.3728x 10-28, μ=1.3732 dB). Information about the charge density distribution of the molecules and their chemical reactivity was obtained by mapping the molecular electrostatic potential surface (MEPs).

*Speaker

The Mullikan atomic charges, molecular electrostatic potential surfaces, electric response properties, dipole moments, electric multipole moments and polarizability of the complex was calculated. The calculations show that the highest positive charge density is collected on the copper atoms (0.921 au for B3PW91 method and 0.927 au for B3LYP methods), while the lowest negative charge density is on the carbon atoms (-0.688 for B3PW91 methods and -0.686 for B3LYP method). Additionally, HOMO and LUMO energy levels and molecular transition energies of the complex [Cu(etim)4Pd(μ-CN)4]n has been calculated by time depended density functional theory with B3LYP and B3PW91 methods with LANL2DZ basis set. The electronic transition energies between the HOMO and LUMO level of the complex were determined as 0.211 eV for both of the calculations (Figure 3).
Keywords: 1-Ethylimidazole complex; Cyanide-bridged complex; Heteronuclear polymeric complex; Copper(II) complex; Structural and vibrational analyses; DFT; B3LYP; LANL2DZ; B3PW91.

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P44: Calcium Oxalate Polyhydrate morphologies from first principles

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One of the research topics of our group is the study of pathological calcifications i.e. the formation of minerals induced by diseases. In this frame, in vivo CaOx crystallization leads to the formation of kidney and urinary stones, constituting a serious health problem to mankind (10% of the population in industrialized countries). Our group is especially interested in the study of the formation and characterization of these in vivo produced calcium oxalate minerals.
Calcium oxalate crystallization yields three main hydrates, i.e. thermodynamically favorable calcium oxalate monohydrate (COM), metastable calcium oxalate dihydrate (COD) and calcium oxalate trihydrate (COT).**1** Monoclinic COM and tetragonal COD are the most commonly found in human stones, plants and fossils.2-4

After an extensive investigation on CaOx kidney stones through FTIR, SEM and PND, our group recently started to investigate the calcium oxalate polymorphs using ab initio quantum chemical methods.7Ab initio calculations based on periodic DFT (Density Functional Theory) enable to determine the crystal structure with high precision, and compare it with experimental X-ray based crystallographic and neutron diffraction methods, but also investigate the theoretically calculated vibrational frequencies of the bulk crystal. This information gives access to simulated IR spectra obtained on perfect (defect free crystals) with high accuracy.

After the study of the bulk, the next step is the theoretical investigation of the different surfaces of the calcium oxalate polymorphs. Indeed, from the bulk crystal structures obtained through ab initio methods one can build for example the low index surfaces. Surface energy of the different surfaces can be calculated and the final crystal morphologypredicted using the thermodynamic Wulff formalism for the construction of the crystals shape. Since the thermodynamic stability depends on the medium in which the surface is introduced, the calculation of the interaction of the calcium oxalate surface with water, urea, and other small molecules will give us the possibility to understand the change in crystal morphology of the final oxalate crystal in its natural medium.The final aim is the prediction of the shape of the kidney stone in its natural medium. On this topic it was shown recently that unusual morphological calcium oxalated dihydrate crystals were obtained in the presence of green tea extract containing catechin.**8**

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High resolution IR spectra will first help us to determine and/or confirm the crystal structure of the polymorphs. Second, the comparison of high resolution IR spectra of the pure calcium oxalate polymorphs as well as with real kidney stone samples with the theoretically obtained spectra might help us to understand and explain quantitatively the composition of an oxalate based kidney stone. And finally ATR measurements will help us to investigate adsorption properties at the molecular level, such as adsorption geometry and energies.

Concerning the investigation of the molecular adsorption properties, the molecular catechin will receive special attention because of their known effect on the kidney stone formation in particular their morphology and composition.

The proposed model crystals and surface models selected will be geometrically optimized using periodic DFT by means of the VASP.5.3 code. On these optimized structures vibrational frequencies and their IR intensities will be calculated, in order to obtain theoretical IR spectra that will be compared with the experimental IR spectra.

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P45: Solvation free energy in protein docking process: a molecular dynamics study

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Water plays an important role in biology. Numerous kinds of biomolecules activate their functions in a hydrated environment, via mechanisms that are strongly influenced by interactions with water. For example, protein folding, protein structural stability, and protein function depend on the dynamics and the (dynamic and/or static) structure of the surrounding water. Recently we observed a large solvation free energy change with a perturbation from native structure of a soluble protein. In this study, we focused the effect of hydration water to the protein-docking system. The solvation free energies were estimated from the trajectory data of classical molecular dynamics simulation of Barnase -Barstar by means of the energy representation method. The free energy profiles along to the distance between van del Waals surfaces of protein subunits indicated that the hydration effect ranged over 8 Å distance. The density distribution of water Oxygen or Hydrogen atom in the MD grid space was investigated for the correlation to free energy. The three dimensional profile of density water was also discussed for the hydration effect.

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P46: Study of coupled oscillators' locking pattern on complex networks

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In the previous study, we observed the phase directionality of the coupled oscillators can be changed due to the coupling function. Then now, we investigate the classification of phase distribution patterns depending on the key parameters in more details. With numerical simulation and mathematical analysis, we obtain the analytic relationship between structural and functional information and phase dynamics.

*Speaker

P47: Computational studies on cyclic imide formation mechanism of glutamic acid residues catalyzed by two water molecules

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Although all of amino acids constituting proteins except glycine have a pair of enantiomers of l- and d-form, only l-amino acids are used for protein biosynthesis. Detection of d-amino acid residues has recently been reported from proteins, and it d-amino acid residues are considered to generate in the process of aging. Almost all of the detected d-amino acid residues are the aspartic acid (Asp). It is believed that the stereoinversion of Asp residues proceeds nonenzymatically via succinimide five-membered ring intermediate. Experimentally, Fujii et al. reported an Arrhenius plot for the succinimide formation in a human αA-crystalline fragment peptide, from which the activation energy can be calculated to be 21.4-28.3 kcal/mol. We studied a stereoinversion pathway of Asp using density functional theory (DFT), and reported that a barrier of the water-assisted stereoinversion pathway were estimated at less than 30 kcal/mol. Among the amino acids constituting proteins, the chemical structures of glutamic acid (Glu) is similar to Asp, however there are few reports that d-Glu residues were obtained from protein. We presumed that the stereoinversion of l-Glu residues proceeds via glutarimide six-membered ring intermediate, and investigated the activation barrier on stereoinversion of Glu residues using DFT calculations. Recently, we performed the DFT calculation of keto-enol tautomerization of glutarimide intermediate, and we reported that there was no significant difference in activation barrier of stereoinversion between succinimide and glutarimide intermediates. In order to investigate the reason why the stereoinversion of Glu residues is less likely to occur compared with Asp residues, we focused on cyclization of Glu residues. In this study, we investigated the activation barrier on glutarimide intermediate formation using DFT calculations. The calculated activation barrier of cyclization of Glu residues is 23.8 kcal/mol, there was no significant difference in activation barrier on stereoinversion of Asp and Glu residues, thus it is considered this reaction can proceed under physiological conditions. The details of the calculation result will be reported on the day.

*Speaker

P48: Free energy profiles of lipid translocation across mixed lipid bilayers: a molecular dynamics study

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Addition of different lipids to membrane largely changes structural and dynamical properties of the membrane, and such changes affect the functions of membrane such as signaling and molecular translocation across the membrane. Especially cholesterol makes membrane dense and changes the state to the liquid-odered phase above around 20 mol% of cholesterol. Such membrane condensing effect also occurs by adding other lipids; ceramide, diacylglycerol and sphingomyelin. However the differences of condensing effects by these lipids and the effects on molecular translocation like lipid flip-flop are not well known yet. In this study, we thus carry out molecular dynamics simulations of mixed binary POPC bilayers with cholesterol, ceramide, diacylglycerol and sphingomyelin and investigate the effects of these lipids on structure and dynamics of the POPC bilayer. We also evaluate the potential mean force (PMF) of POPC translocation across the mixed bilayer by free energy calculations and discuss the differences of condensing effects on the lipid flip-flop in the membrane.

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P49: Prediction of three-dimensional structures of histone deacetylase 1 complexed with romidepsin and its analog

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Romidepsin is one of the anticancer drug, which inhibits the histone deacetylase (HDAC) in human cell. Recently, we found the inhibitory activity of romidepsin and its analog for phosphoinositide 3-kinase (PI3K). Thus, romidepsin and its analog are promissing HDAC/PI3K dual inhibitor and novel anticancer drug. Although the predicted three-dimensional (3D) structures of the complexes between PI3K and romidepsin analog have been already reported, the 3D structures of HDAC-inhibitor complexes were not predicted. In this study, the complex structures were predicted by using computational docking and molecular dynamics (MD) simulations. Because romidepsin and its analog inhibitor, FK-A5, are large cyclic molecules, large numbers of conformers can be obtained for these molecules by the computational chemical treatment. For the conformational search, LMOD method was used for the preparatory calculations of computational docking by GOLD, in which conformational search is insufficiently performed for large (more than six-membered) ring. The docking poses were extracted by comparing romidepsin and FK-A5, because similar compounds are recognized by proteins in similar binding modes. The MD simulations were conducted for the selected docking poses, and the protein-ligand interactions were analyzed. The computational results are expected to be useful for the rational drug designs of HDAC inhibitors.

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P50: Effect of the Arg456His mutation on the three-dimensional structure of cytochrome P450 1A2 predicted by molecular dynamics simulations

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Cytochrome P450 1A2 (CYP1A2), which is the major drug-metabolizing enzyme among CYPs, is known to have many variant alleles. The genetic polymorphism of CYP1A2 may cause individual differences in the pharmacokinetics of medicines. One of CYP1A2 variants, CYP1A2.8 (Arg456His mutant) has been reported to have decreased enzymatic activity. The Arg456His mutation is located at the most conserved motif (FXXGXRXCXG) and the arginine is suggested to fold and locks the Cys-pocket in proper position by interacting with the propionate group of the heme molecule. In our previous work, in order to understand the reason why Arg456His mutant lost the enzymatic activity, we constructed the Arg456His mutant with the hydrogen on the epsilon nitrogen of the histidine (HIE) and performed 300-ns MD simulation [1]. HIE would be suitable for the interaction with the surrounding residues including the heme molecule. After MD simulation, the Arg456His mutant with HIE showed large differences on the static structure as well as the flexibility compared with the wild type, which would be the reason of the decreased activity. In the present study, in order to consider the effect of the protonation state of the histidine, we constructed additional Arg456His mutant structure with positive charged histidine (HIP) which would have more electrostatic interaction with the surrounding residues than HIE. We performed 300-ns MD simulation at 300 K for the Arg456His mutant with HIP and compared the static structures, the structural flexibilities, and the interaction. The minimizations and MD simulations were conducted using the Amber 12 program, and the tleap module of AmberTools was used for construction of the mutants. We employed our previously determined force field parameters around the heme iron [2], and the AMBER ff12SB force field was adopted for the amino acids. As a result, the static structures and the structural flexibilities of two Arg456His mutants were dissimilar because of difference between HIE and HIP. Though the root mean square deviation (RMSD) of the Arg456His mutant with HIE showed the existence of

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metastable state during the 300-ns MD simulation [1], the RMSD of that of HIP did not show the metastable feature. Moreover, the structural flexibilities predicted by measuring the root mean square fluctuations (RMSFs) were not same. These results indicate that the protonation state of the His456 residue has large influence on both of the static structure and the structural flexibility.

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P51: Molecular dynamics study of interaction between PACAP (6'–38') and N-terminal extracellular domain of the human splice variant hPAC1-R-short aiming at development of neuropathic pain medicine

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The chronic pathetic pain represented by postherpetic neuralgia and sciatica is caused by external injury of the central and peripheral nerves. The pathogenic mechanism of the chronic neuropathy has not been elucidated and existing analgesics such as non-steroidal anti-inflammatory agents are not helpful enough for the chronic pain relief. In the nervous conduction of pain, pituitary adenylate cyclase-activating polypeptide (PACAP), a peptide hormone consisting of 38 or 27 amino acid residues, acts as a neurotransmitter or a nerve modulate factor. Therefore, the PACAP selective receptor, pituitary adenylate cyclase-activating polypeptide type I receptor (PAC1-R), is a potential target for the treatment of the neuropathic pain. That is, inhibition of interaction between PACAP and PAC1-R is expected to restrain the neuropathic pain and lead to the development of a new strong painkiller. Recently, the structure of PACAP (6'–38') in complex with the N-terminal extracellular (EC) domain of the human splice variant hPAC1-R-short (hPAC1-RS) was reported [1]. PACAP (6'–38') is a shorter analogue of PACAP-38 and is known to act as a potent antagonist. Therefore, detailed investigation on the interaction between PACAP (6'–38') and N-terminal EC domain of hPAC1-RS would be informative for structure-based drug design of the PAC1-R inhibitor. In this study, we conducted the molecular dynamics (MD) simulation to investigate solution structure of the complex of PACAP (6'–38') and N-terminal EC domain of hPAC1-RS in detail. Using the Amber 14 program, 80 ns MD simulation of the complex was performed at 300 K under constant pressure. In order to understand the important residues for the interaction, hydrogen-bond analysis between hPAC1-RS and PACAP (6'–38') was performed using 60-80 ns MD trajectory. As a result, the analysis revealed some strong hydrogen bonds between acidic residues of hPAC1-RS and basic residues of PACAP (6'–38'), suggesting that these residues are important for the interaction of hPAC1-RS and PACAP (6'–38').

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P52: Structural differences of the ligand binding pockets between estrogen receptor alpha and beta

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The estrogen receptor (ER) is the member of the nuclear receptor superfamily. Inhibition of ERα is an effective therapeutic strategy in breast cancer remedy. In contrast, ERβ is presumed as the drug target of autoimmune diseases. Many experimentally determined conformations of ERα and β have been reported, however their structures are different from each other because of various ligands. To develop ERβ selective ligands, the structural differences between ERα and ERβ are to be clarified in detail. In this study, we carried out the structural bioinformatics studies for the 3D structure of ERs retrieved from PDB. 48 structures registered in PDB were analyzed by HBOP and HBSITE which were the programs developed by us to identify the ligand binding cavities in proteins. These structures clustered by the shapes, sizes, and locations of the ligand binding pockets. In addition, the shapes of C terminal domains of ERs were used for clustering, which are known as "agonist form" and "antagonist form." We classified 27 entries of ERα into 5 clusters and 21 entries of ERβ into 7 clusters, thus, all ER structures were classified into 12 clusters. Differences of the pockets and hydrogen bonds with ligands were observed between ERα and ERβ, however, there are differences in the same ER species. The results indicate that ERs are structurally flexible and the structures are affected by the ligands.

*Speaker

P53: Fickian Yet Non-Gaussian Behaviour: A Dominant Role of the Intermittent Dynamics

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We present a study of the dynamics of small solute particles in a solvent medium where the solute is much smaller in size, mimicking the diffusion of small particles in crowded environment. The solute exhibits Fickian diffusion arising from non-Gaussian van Hove correlation function. Our study shows that there are at least two possible origins of this non-Gaussian behaviour. The decoupling of the solute-solvent dynamics and the intermittency in the solute motion, the latter playing a dominant role. In the former scenario when averaged time long enough to explore different solvent environments the dynamics recovers the Gaussian nature. In case of intermittent dynamics the non-Gaussianity remains even after long averaging and the Gaussian behaviour is obtained at a much longer time. Our study further shows that only for intermediate attractive solute-solvent interaction the dynamics of the solute is intermittent. The intermittency disappears for weaker or stronger attractions.

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P54: DFT study of the vibrational and electronic properties of InAs nanowires

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Binary semiconductor nanowires have attracted much attention due to their attractive properties for applications in the electronics and energy fields, indium arsenide nanowires (InAsNWs) are especially interesting due to their narrow band gap and high carrier mobility, which have led to their applications in photodetectors and transistors. There are multiple experimental investigations on the properties of InAsNWs, however there are seldom theoretical ones, especially on their vibrational properties. In this work the vibrational and electronic properties of InAsNWs were studied using a first principles density functional theory and the supercell scheme [1]. The nanowires were modelled by removing atoms outside a circumference on the [001] direction, where all the surface dangling bonds are passivated with H atoms. The results show that the expected shift of the highest optical vibrational modes to lower frequencies due to the phonon confinement is lessened due to bending modes of the surface H. It was also observed that the electronic band gap broadens as the nanowire diameter decreases. These results could be important for future characterization of these nanowires.
Acknowledgments:

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P55: Modelling of the quantum confinement effects on the optical properties of GaSb nanowires

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Recently binary semiconductor nanomaterials have attracted much attention due to their attractive properties, gallium antimonide nanowires (GaSbNWs) are specially interesting due to their high hole mobility and direct band gap that makes them suitable for optoelectronic applications and photodetectors. There are only a few theoretical and experimental studies on the properties of GaSbNWs and none of their optical properties (to the best of our knowledge). In this work the electronic and optical properties of GaSbNWs are studied using the first principles density functional theory and the supercell scheme [1], where the nanowires are modelled by removing atoms outside a cylinder on the [111] direction of an otherwise perfect GaSb crystal, all surface dangling bonds are passivated with H atoms. Results show that as the nanowire diameter decreases the imaginary part of the dielectric function suffer a shift to higher frequencies while the electronic band gap increases, these results are in accordance to the quantum confinement scheme. This study could be of great importance for the applications of these nanowires for optoelectronic applications.
Acknowledgments:

This work was partially supported by multidisciplinary projects SIP-IPN 2016-1771 and 2016-1770 by Instituto Politécnico Nacional

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P56: Metal-porphyrin-like graphenes for selective ammonia capture

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We performed a computational search for selective ammonia (NH3) capture by using transition metal (TM)-porphyrin-like graphene based on first principles thermodynamics. We find that NH3 molecules can selectively adsorb TM atom under humidity condition even at room temperature and low pressure. Using equilibrium thermodynamics, we conformed that Sc-, Ti-, and V-porphyrin-like graphenes can selectively capture NH3 under mixed gases with water and the capacity reach _˜5 mmol/g at room temperature under low pressure. This result allows us to discover novel promising selective ammonia capture materials based on TM at ambient conditions.

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P57: Structural Rietveld refinement and vibrational study of ZnxCo1-xFeO4 spinel ferrites

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Spinel ferrites with the general formula ZnxCo1-xFeO4 (0 £ x £ 1) were synthesized by the ceramic technique and characterized using X-ray diffraction, FT-Infra Red and Raman spectroscopy. The X-ray diffraction pattern confirms that the mixed ferrite samples are in cubic spinel structure, which is further validated by Rietveld refinement in the space group Fd3m. The lattice parameters, bond lengths, crystallite size and density have been determined by means of Rietveld analysis. From FT-Infra Red band frequencies, the force constants Kt and Ko for tetrahedral (A) and octahedral (B) sites respectively, have been calculated and compared with the bond lengths trend obtained by Rietveld refinement. For all compositions, Raman spectra show the five active modes A1g + E1g + 3 T2g of the motion of O2- ions and both the A-site and B-site ions.

*Speaker

P58: I-V Characteristics of Graphene Nanoribbon/h-BN Heterojunctions

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We present the first principles calculations for electrical properties of graphene sheet/h-BN heterojunction(GS/h-BN) and graphene nanoribbon/h-BN heterojuctions(NR/h-BN). which are carried out by the density functional theory method and the nonequilibrium Green's function techniques. Especially, nanoribbon with two parallel arrays of h-BNs has unique properties. Because the h-BNs are wide-gap semiconductors, the two arrays show the quantum double barrier tunneling effect. The graphene sheet and the (3n-1)-family of armchair type NR are known as metallic nanomaterials. Settling two arrays of h-BN into the nanomaterial, the double barrier tunneling effect makes the transmission function very spiky and also leads step-wise I-V characteristic rather than negative resistance of much larger ordinary semiconductor.

*Speaker

P59: The driving force for the charge ordering in the nickelates

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An almost ubiquitous charge ordering is seen in the rare-earth nickelates of the form RENiO3 (RE=rare-earth), with the exception of LaNiO3. We show that the charge ordering (more precisely, two-sublattice bond disproportionation) in the rare earth nickelate perovskites is intimately related to a negative charge transfer energy. By adding an additional potential on the Ni d states we are able to vary the charge tranfer energy and compute relaxed structures within an ab-initio framework. We show that the difference in Ni-O bond lengths and the value of the ordered state magnetic moment correlate with the charge transfer energy and that the transition to the bond-disproportionated state occurs when the effective charge transfer energy becomes negative.
This is work done in collaboration with Sagar Sarkar, Basudeb Mandal, Shishir Kr. Pandey, Cesare Franchini, A.J. Millis and D.D. Sarma.

*Speaker

P60: Effect of p- and n-type dopant on optoelectronic properties of 2D-HfS2

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2-Dimentional (2D) layered materials display interesting, extraordinary electronic properties and significance for future high-performance electronics and optoelectronics device manufacture. In the present paper, we have study effect of p- and n-type doping on electronic structure and optical properties of TMDs 2D-HfS2. Our calculations are based on density functional theory (DFT) using the PBE functionals by VASP software. Furthermore, we have symmetrically investigated the structural and optical properties of 2D-HfS2 by doping of p- and n-type dopant. We observed possible changes in dielectric function and optical absorption spectrum due to changes in electronic band structure and band gap. All these theoretical contemplations are needed to shed light on fabricating optoelectronic devices using 2D TMDs HfS2 material.

*Speaker

P61: Mathematical model of novel concept of optical image registration in wide spectral range by piezoelectric microresonators

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The majority of modern systems of optical image registration exploit matrixes of photosensitive semiconductor elements. However, in case of measuring high-intensity light flux it has to be strongly attenuated, as semiconductor elements can be easily overexposed and even damaged. Moreover, semiconductor optical sensors can work efficiently only in certain wavelength range as a rule of several hundred nanometers. In present paper, we introduce novel concept of optical image registration free of compulsory attenuation using matrix of transparent piezoelectric crystals. Each crystal represents direct sensor of incident power level of electromagnetic radiation. This system operates in wide spectral range restricted only by transparency bandwidth of applied crystals.
For measuring the optical power interacting with certain matrix element we employ piezoelectric laser calorimetry technique [1]. This allows measuring of optical power part absorbed by piezoelectric crystal exploiting dependence of crystal piezoelectric resonance frequencies on crystal temperature, which is increased under crystal irradiation. Piezoelectric resonances are observed by measuring crystal response to the applied radiofrequency electric field when its frequency corresponds to one of the crystal internal vibration modes. Preliminary performed calibration of piezoelectric resonance frequencies shift in condition of uniform heating allows determination of somehow averaged temperature of irradiated crystal [1]. Absorbed power can be calculated using crystal temperature kinetics derived from measured resonance frequency change in time. In order to obtain the absolute value of optical power transmitted through certain matrix element the dependence of its optical absorption coefficient on wavelength should be predetermined.

When using FEM for frequency domain analysis of piezoelectric response of matrix single element, the result of resonance frequencies calculation strongly depends on sample dimensions as well as involved mechanical boundary conditions and nonuniform temperature distribution. Moreover, in case of inhomogeneous electric field distribution, Q-factor of piezoelectric resonance depends on crystal position in space. It was proven experimentally that these facts enable distinction of resonance signals from different matrix elements in measured overall response radiofrequency spectrum. Calculated spectrum responce is in good agreement with measured one.

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P62: The thermodynamic properties and bonding feature of the some B2 rare-earth intermetallic compounds: first principal study

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The full-potential linearized augmented plane wave (FP-LAPW) method has been employed within the generalized gradient approximation (GGA) to investigate the structural and thermo-elastic properties of some rare earth intermetallics such as YAg, YCu, HoCu, LaAg, LaZn, and LaMg compounds. The calculated ground state properties such as lattice constants, bulk modulus and elastic constants agree well with the experiment. For HoCu and LaZn compounds, the thermodynamic properties are predicted [1] via the quasi-harmonic Debye model, using to predict the low-temperature behavior of the crystal. For the first time, the numerical estimation of the thermal properties is performed for these compounds and still await experimental confirmations. In addition, the chemical bonding of these compounds has been investigated in the light of topological analysis approach based on the theory of atoms in molecules (AIM).

Key words: Intermetallic compounds; Ab-initio calculations; Electronic structure; Elastic properties; Thermal properties.

[1] A. Sekkal , A. Benzair , T. Ouahrani , H.I. Faraoun , G. Merad , H. Aourag , C. Esling Mechanical properties and bonding feature of the YAg, CeAg, HoCu, LaAg, LaZn, and LaMg rare-earth intermetallic compounds: An ab initio study.Intermetallics 45 (2014) 65-70

*Speaker

P63: Crystal Structures, Electronic, Vibrational and Optical Properties of few Single Monolayer of SnH

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Single-layer Stannane (SnH) structures have been explored using evolutionary algorithms combined with first-principles methods. We reported hexagonal types of some monolayer crystal of chair, stirrup and boat type along with their band structure and PDOS. The chair SnH is the found direct band gap at Γ-point and other structure are have both direct and indirect band-gap. The band gaps of mono layer of SnH structures are calculated to lie between 0.74 eV to 1.40 eV using the hybrid HSE06 functional, and they aremdependent on the crystal structure geometry. Vibrational properties also calculated for crystal stability. It is heartening to note that the developed material is identified as direct and indirect band gap semiconductor which are predictable to have high solar energy conversion efficiency or may be useful in opto-electronics application.

*Speaker

P64: Structural, electronic and magnetic properties of GdFeSi : DFT+U study

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The structural, electronic and magnetic properties of the intermetallic compound GdFeSi have been studied using both Local Density Approximation (LDA) and LDA+U within the framework of density-functional theory (DFT). At equilibrium, spin-polarization calculations with Hubbard approximation were performed and show that GdFeSi shows a typical metallic behavior and carry magnetic moment. The calculated atomic positions, lattice parameters, bulk moduli, electronic structure and magnetic moments agree well with experimental and the unique other theoretical results. Finally we remarked that the spin-polarization and the Coulomb repulsion potential U play crucially important role in determining the electronic, magnetic and structural properties of this magnetocalific compound.

*Speaker

P65: Computational Studies of The Development of GLI-associated oncogene inhibitory Synthetics

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In cancer cells, binding of the Hh protein to the membrane receptor patched 1 (PTCH) releases its inhibitory effect on Smo. Activated Smo further transduces downstream cascades to activate the glioma-associated oncogene (GLI) family of transcription factors Recent papers reported that GLI has been considered as a promising target for selective cancer therapy. We performed *in silico* screening of dibromosesamine (DBSE) and 3'-methoxy-3'',4'' (methylenedioxy)-2,5-epoxylignan-4'-ol-6-on (DMEO) against GLI1, GLI3, 2GLI and Smoothened (SMO) as targets. The docking protocols used PLANTS (Protein-Ligand Ant System) software and evaluated parameters were included the interaction energy and hydrogen bond. A crystal structure of cyclopamine binds to 2GLI was used as the reference structure at the score of root mean square deviation of 1.614 Å. As a result, DBSE and DMEO share similar interactions with protein residues within the 2GLI binding pocket and have potential to inhibit GLI binding. Both synthetics did not bind to receptors GLI1, GLI 3 and SMO. The best conformation of DBSE-bound to 2GLI was on the amino acid of His 129. Meanwhile, DMEO-bound to 2GLI has the best conformation on the amino acid of Arg 162, Arg 183, Leu 184 dan Lys 188. The surface characteristics of the particles were observed by scanning electron microscopy (SEM) while crystalline peaks were observed in the diffraction patterns of X-Ray Diffraction (XRD).

*Speaker

P66: BAND GAP TUNING OF ALUMINA BY SURFACE ADSORPTION OF II GROUP ELEMENTS: A DFT STUDY

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We present a density functional theory study of the adsorption reactions of p-group atoms onthe (0001) surface of the α-Al2O3. In this work, we work on α-Al2O3 (Corundum) monolayer and we found that the band gap 4.58 eV has been reduced compare to bulk structure 6.24 eV,which is tuneable from insulator to semiconducting nature by adsorbing different solid andgas adatoms by using first-principles calculations. The effect of adsorption of p-group atomssuch as metal atoms- B, C and gas atoms -N,O,F owing physisorption and chemisorptions process on the alumina (Al2O3) surface which have been systematically concluded byadsorption properties using density functional theory (DFT). Due to the hybridization of adsorbate selected elements, they help to tune the electronic properties along to the n-typeand p-type direction, which light up the new way to develop cheap and possible device. Presented adsorption process is also very clearly defined by adsorption energy, electronic band structure, projected density of state (PDOS), and electron localised function (ELF). We thus light up the way to producing a tuneable alumina band gap by adsorbing adatoms, whichmay play an important role in the utilisation of alumina in future alumina -based electronicnano-devices.

*Speaker

P67: Development of Reliable Interaction Potential for and Results of Molecular Dynamics Simulations of ZrO2 Film Growth

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Thin films of ZrO2 are of high interest due to a wide range of useful technological properties. In this contribution the growth of ZrO2 is studied by atom-by-atom molecular dynamics simulations, focused on intrinsic process parameters such as the energy (E) and energy distribution function (EDF) of arriving atoms or the surface temperature (T).
The first part deals with the development of an interaction potential for a realistic description of atom-by-atom ZrO2 growth. Owing to the fact that for many metal oxides including ZrO2 only full-charge (Zr+4 and O-2) interaction potentials are available in the literature, special attention is paid to the effect of the Zr and O elemental charges. Parameters of the short-range part of the Buckingham interaction potential leading to experimental lattice parameters and formation energies have been identified in a wide range of elemental charges. Simulations reveal that the structures grown using the presently available full-charge interaction potentials are in contradiction with the experiment (the atoms have too low coordination numbers). Correct partial charges and potential parameters leading to experimentally relevant structures (with correct coordination numbers) have been identified [1].

The second part shows how do the film densification, crystal nucleation and uninterrupted crystal growth depend not only on E delivered into the growing films (i) per fast atom (ion) or (ii) per any atom, but especially (iii) on the EDF (namely the fraction of fast atoms in the particle flux) and (iv) on the mass of fast atoms (Zr or O). On the one hand, the nucleation of c-ZrO2 (the most desired phase) is T-dependent and requires (in order to take place on a short time scale) high E. On the other hand, the growth of previously nucleated (or epitaxial growth of) c-ZrO2 is much easier, T-independent, and highly dependent on the EDF. Optimum EDFs which allow uninterrupted crystal growth at as low E delivered into the growing films as possible are characterized by (i) narrow EDF and (ii) high momentum delivered into the growing films (i.e. the combination of fast Zr and slow O leads to better densification and crystallinity than the opposite) [2].

The results are of methodological importance for the interaction potential development, facilitate defining new synthesis pathways for ZrO2, and constitute phenomena which may be relevant for other coating materials (isostructural HfO2 at the first place) as well.

Acknowledgment

*Speaker

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P68: Band Gap of BN co-doped Graphene, first-principles investigation.

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Chemical doping is a well-known method used to modify the electronic properties of materials. In this work, using ab initio density functional theory calculations, we have investigated the effect of graphene co-doped with boron and nitrogen atoms at low concentration. The results for the electronic structure of doped graphene predict that co-doped graphene band gaps can vary over an order of magnitude, for the same BN concentration, depending on the system morphology. This result was described by a tight-binding model. Also, It was shown that the band gap size is affected by the lattice deformation.

*Speaker

P69: High Pressure Structural Phase Transition in NdX (X=P, As, Sb): A Density Functional Theory Study

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The structural and phase transition properties of NdX (X = P, As, Sb) under high pressure have been investigated using an *ab-initio* full potential linear augmented plane wave plus local orbitals approach within the framework of density functional theory as implanted in the WIEN2k package. In this approach the generalized gradient approximation is chosen for the exchange-correlation functional energy optimization for calculating the total energy. At ambient conditions NdX stabilize in NaCl (B1 phase) structure. Under compression, it undergoes first-order structural transition from *Fm-3m* to *P4/mmm* (body centre tetragonal) phase at 30.0, 24.06 and 15.1 GPa which is found to be in good agreement with the available experimental data 30.0, 24.2 and 15.0 GPa respectively. The structural properties *viz.*, equilibrium lattice constants, bulk modulus and its pressure derivative and volume collapse are also calculated and compared with previous calculations and available experimental data.

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P70: The Effects of Vacancy-Defect, Adsorbent and Li Dopant on Electronic and Magnetic Attributes of MoO3 (010) Bilayer: A First-Principles Study

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In this work, a systematic DFT calculation was carried out to investigate the electronic features of MoO3 (010) bilayer under different situations of a) Molybdenum and oxygen vacancies, b)adsorption of gas molecules on it, c) adsorption and intercalation of lithium atoms. The possibility of obtaining magnetic phase from native defects in orthorhombic MoO3 was explored, whereas Mo vacancy provides the transition of the insulating molybdenum trioxide into a metallic-like phase and changes the electronic transport. Furthermore, we studied the adsorption of gas molecules and the most stable configurations, magnetism, adsorption energies and electronic properties were thoroughly discussed. Due to the calculated adsorption energies, it was explored that MoO3 bilayers exhibit suitable parameters for serving as a gas sensor. Moreover, Lithium adsorption on the both topmost Mo and O sites shifts the Fermi level into the MoO3 conduction band and makes the n-type semiconducting.

*Speaker

P71: First Principle Study on the Structure, Electronic and Optical Properties of MoS2 /AlN Hybrid Bilayer

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The first principle investigation on the structural and opto-electronic properties of heterobilayer MoS2 /AlN
has been performed using plane wave pseudo potential method under density functional theory. A direct band gap of

0.96 eV is found for the MoS2 /AlN bilayer system. The calculated physical parameters of MoS2 /AlN are noticed to be

very close to bulk MoS2 and compare well with existing other theoretical results. The calculated projected density of states

(PDOS) may be useful for understanding the nature of band gap. The optical properties of the MoS2 /AlN layer such as

dielectric function, reflectivity R(ω), absorption coefficient I(ω), energy-loss spectrum L(ω), and the refractive index
n(ω) are calculated for parallel polarizations.

*Speaker

P72: High-throughput screening of carbon-capturing materials with ab initio and thermodynamic calculation

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Nanostructured materials, such as zeolites and metal-organic frameworks, have been considered to capture CO2. However, their application has been limited largely because they exhibit poor selectivity for flue gases and low capture capacity under low pressures. We perform a high-throughput screening for selective CO2 capture from flue gases by using first principles thermodynamics. We find that elements with empty d orbitals selectively attract CO2 from gaseous mixtures under low CO2 pressures (_˜10–3 bar) at 300 K and release it at _˜450 K. CO2 binding to elements involves hybridization of the metal d orbitals with the CO2 π orbitals and CO2-transition metal complexes were observed in experiments. This result allows us to perform high-throughput screening to discover novel promising CO2 capture materials with empty d orbitals (e.g., Sc– or V–porphyrin-like graphene) and predict their capture performance under various conditions. Moreover, these findings provide physical insights into selective CO2 capture and open a new path to explore CO2 capture materials.

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P73: First-Principles Approach of the Structural, Electronic and Dynamical Properties of SixGe(1-x) ($0 \leq x \leq 1$), SiC, GaX (with X = P, As, Sb): A Study of the Hybrid Functionals Performance.

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The electrical properties of semiconductors, such as the concentrations and mobilities of the charge carriers, are strongly influenced by the types of dopants and defects inserted or formed during the synthesis of materials. In the context of photovoltaics, these defects can degrade the efficiency and durability of solar cells. First-principles microscopic theory, implemented e.g. via an accurate but very time consuming method such as GW, can give a clue to how the crystal structure influences electronic (optical) characteristics. An interesting alternative can be provided by so-called hybrid functionals elaborated within the density functional theory. Several models and parameterizations have been suggested for practical use; they differ in the percentage of the Hartree–Fock exchange incorporated in the exchange-correlation schemes. In this work, the performance of different functionals has been compared in what regards their ability to correctly describe electronic, structural and dynamical properties of IV(Si)-IV and III–V semiconductors. For each compound, we determined the best combination of Hartree–Fock exchange with different LDA and GGA functionals in order to obtain a good description of their band structures. In that case, we show that other properties, such as the lattice parameters, phonons, dielectric and elastic constants, have also a good agreement with experimental data. Additionally, simulations with different software have been done in order to examine the transferability of the obtained functionals.

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P74: Hard-Sphere Melting and Crystallization with Modern Hybrid Algorithms

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The hard disk/sphere systems are one of the most important models to investigate fundamental problems in the field of statistical physics. From the numerical point of view, simulation results on the melting/crystallization of this model were one of the historical milestones. After pioneering works on this issue by Monte Carlo(MC) and molecular dynamics (MD) methods in 1957 [1], enormous implementations of algorithms and a wide variety of applications including general potentials have been investigated. Here, we revisit the melting and crystallization problems in the hard disk/sphere systems with modern algorithms, especially for Event-Chain MC [2] and Event-Driven MD [3], where we propose the"Hybrid Scheme," namely, Event-Chain MC for equilibration and Event-Driven MD for calculation of dynamical properties [4]. This paper addresses applications of those methods in the two- and three-dimensional melting/crystallization [5,6] including the binary mixture glassy systems [7].

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*Speaker

P75: Investigation of electrode passivation phenomenon in Li-O2 batteries by means of macrokinetical modeling of RRDE experiments.

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Li-O2 batteries are a promising technology that potentially can deliver energy density up to 1000 Wh/kg, which is several times higher than that of li-ion cells. The benefit arises because the discharge product Li2O2 filling the cathode is much lighter than heavy metal oxides used in li-ion cells. Unfortunately, actual discharge capacities of Li-O2 cells are well below expectations that is associated with electrode surface passivation as bulk Li2O2 is an insulator. However amorphous and polycrystalline Li2O2 can exhibit sufficient conductivity due to defects and grain boundaries. Thus resistance of the layer would depend on the growth conditions. The growth of the passivating film may proceed according to two channels: electrochemical reduction of intermediate product LiO2 (generated upon oxygen reduction) and chemical disproportionation (2LiO2 -> Li2O2 + O2).
Rotating ring-disk electrode (RRDE) is a powerful tool that enables to control specie flows and detect short-lived reaction products such as LiO2. Species concentration near the electrodes surfaces can be calculated to perform quantitative analysis of the electrochemical reaction rate and standard potential. Unfortunately, the conventional analytical description of RRDE experiment can not be applied in case of Li-O2 system due to passivation phenomenon.
In this work we obtain the passivation rate as a function of time by solving the inverse problem and incorporate passivation effect into the macrokinetical model of RRDE experiment, that allowed us to calculate the true LiO2 concentration distribution. The results reveal that the electrode surface passivation rate is proportional to the intermediate concentration while independent of the disk cathodic current. Furthermore, we propose an approach to differentiate the passivation rate originating from electrochemical reduction of LiO2 and disproportionation. The extracted dependence of the passivation rate on the intermediate concentration can be used to optimize pore structure of Li-O2 cathode in order to achieve higher cell capacities.

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P76: STRAIN-INDUCED MODULATION OF 2D TRANSITION METAL DICHALCOGENIDES HOMO AND HETEROSTRUCTURE: PREDICTION FROM COMPUTATIONAL APPROACH

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The ultimate goal of this research work using density functional theory calculations, the electronic properties, magnetic and phonon band structure of two-dimensional (2D) bilayer systems of transition metal dichalcogenides (TMD) investigated. Some of TMDs investigated for the biaxial tensile and compressive strain on homo and hetero structure of NbX2 (X = S, Se, Te) influenced by magnatism with a ferromagnetic character cause of the focused impacts of through- bond interaction and also through-space interaction. In whole mechanism of the system, 4d orbital of Nb transition atom play significant role of this exchange on transition of spin moment concept. The raised magnetic moments have been remarkable increased or decreased by the tensile and compressive strain, even affecting a half-metallic and semiconductor properties by the strong spin polarization near the Fermi level. We assume that our calculated outputs might suitable for spintronics-related technologies such as memory and quantum-computer devices are considerable. This would light up a new direction to find out the spintronics in two-dimensional nanostructures.

*Speaker

P77: Molecular simulation of aqueous electrolytes in nanoporous carbons: Blue Energy and water desalination

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When fresh water comes into contact with salty water, a considerable amount of energy is dissipated. Conversely, the desalination of sea water requires a lot of energy. Current processes exploiting this difference in osmotic pressure are based on transport through membranes, with limited efficiency. A new approach has recently been proposed to harness this "blue energy", thanks to the charge / discharge of electrodes in electrolytes with high / low salt concentration. The use of nanoporous carbon electrodes seems promising, but the traditional models (such as Poisson-Boltzmann) used to determine the relevant quantities do not apply in this case where molecular interactions play an essential role. We overcome this difficulty by performing molecular dynamics simulations of nanoporous carbon electrodes in the presence of an aqueous electrolyte. We evaluate the electrical capacity and the amount of ions adsorbed inside the electrodes as a function of the potential difference between the electrodes. In addition, these simulations should allow us to understand the microscopic mechanisms leading to the storage of the charge, the effect of the structure of the carbon electrode, the salt concentration in the electrolyte and the chemical nature of the salt. We will also determine the diffusion coefficients of water and ions and electrical resistance of the solution inside the electrodes.

*Speaker

P78: New non-linear computational approach to analysis, modelling and prediction of chaotic variability of atmospheric radioactive radon 222Rn concentration in atmosphere environment

Vasily Buyadzhi * [1], Olga Khetselius [1], Alexander Glushkov [1], Yuliya Dubrovskaya [1]

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We firstly present a new mathematical formalism to analysis, modeling and prediction of the environmental radioactivity dynamics at whole, and chaotic time series of the radionuclide dynamics in particular. It inlcuded a qualitative analysis of dynamical problem of the typical environmental radioactivity dynamics, reconstruction of the phase space with using methods of correlation dimension algorithm and false nearest neighbor points, determination of the dynamic invariants of a chaotic system, including the global Lyapunov exponents, the Kaplan-York dimension dL , Kolmogorov entropy etc. The forecasting block contains new (in a theory of environmental radioactivity dynamics and environmental protection) methods and algorithms of nonlinear prediction such as methods of predicted trajectories and neural networks modelling [1-3]. As an illustration, there are firstly presented the results of analysis, modeling and forecasting the radon atmospheric concentration dynamics in the Southern Finland (2000-2006) and Chester, New Jersey, USA (1978) using the data from natural measurements from Env. Measurements Lab. and Goddard Institute of Space Studies and Finland Meteorological Institute [4,5]. In particular, for the Southern Finland region the long-term 222Rn data were collected at the SMEAR II station during 2000–2006 [4]. The daily mean atmospheric radon concentration followed a log-normal distribution within the range $<$ 0.1–11 Bq m–3, with the geometric mean of 2.5 Bq m–3 and a geometric standard deviation of 1.7 Bq m–3. In spring, summer, autumn and winter, the daily mean concentrations were 1.7, 2.7, 2.8 and 2.7 Bq m–3, respectively. The presented results (correlation, strange attractors dimensions, dynamical and topological invariants, Lyapunov's exponents, Kolmogorov entropy etc) show that the application of a chaos theory methods to analysis of the time series of the radon concentrations in the atmosphere is quite effective from both theoretical and practical viewpoints and allows quite elegantly and efficiently to give adequate prediction of the atmospheric radon temporal fluctuations dynamics. The carried out complex of the non-linear mathematical chaos-dynamical and multifractal models is of a great importance and effectiveness for analyzing and forecasting a transfer of the radionuclides (including radon) in the areas for which relevant data on radioactive contamination very scarce. Using the theory of fractal sets, chaos, dynamic systems allow to reliably predict and calculate the evolutionary

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dynamics of fluctuations of the radionuclides concentrations in different environments (atmosphere, soils, hydrosystems).

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P79: New computational approach to modelling dynamics of air ventilation and forecasting pollutant concentrations temporal dynamics for city's atmosphere

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We present a new generalized computational approach to analysis and modelling the natural air ventilation in the atmosphere of the industrial city, which is based on the Arakawa model, modified to calculate the current involvement of the ensemble of clouds, and hydrodynamical forecast model (with correct quantitative accounting for the turbulence in an atmosphere of the urban zone). The method allows to calculate the convection parameters and shifting cumulus cloud ensemble from surrounung regions. An advanced computational methods for modelling an unsteady turbulence in the urban area are developed and presented too [1]. For the first time the methods of a plane complex field are applied to calculate the air circulation for the cloud layer arrays, penetrating into the territory of the industrial city. We also consider the mechanisms of transformation of the cloud system advection over the territory of the urban area.
Besides, we present new computational complex approach to studying and forecasting evolutionary dynamics of the environmental statistical systems, based on the combined using the non-linear analysis methods and chaos theory such as the wavelet analysis, multi-fractal formalism, mutual information approach, correlation integral analysis, false nearest neighbour algorithm, Lyapunov exponent's analysis, surrogate data method, stochastic propagators method, memory and Green's functions approach (in version [1]; We identify the concentration space-temporary evolution dynamics for CO2, CO, NO2 , SO2 in the atmosphere of industrial cities in order to reveal the possible chaos in the hourly time series at several sites in Amsterdam, Gdansk and Odessa during the 2003-2009. We present new prediction computational model to forecasting the atmospheric pollutants evolutionary dynamics (new "Geomath" technology). The simple way to identify the chaos in time series is as follows: (1) To determine time delays, the concept of mutual information is used; (2) To determine attractor dimensions, it is used the correlation integral method and false nearest neighbours algorithm; (3) To refine the data, we use surrogate data sets; (4) we evaluate the Lyapunov's exponents as the dynamic invariants of chaotic system. In spite of the fact that the correlation integral method provides the relatively small attractor dimensions, both the surrogate data method and the false nearest neighbours algorithm assert that the more reliable dE for all datasets is 6. Such a value for the embedding dimension is comparatively large, but still indicates the presence of low-D chaos in the series. Also, two positive Lyapunov exponents validate the previous outcome. The sum of

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positive Laypunov exponents is the Kolmogorov entropy which is in turn inversely proportional to the predictability limits. In our case, these limits vary from about three to four days. We develop a new non-linear prediction method and compare the predicted values with both last one hundred data and nine hundred random data in the series. As an example, the real and predicted concentrations of CO2, CO, NO2 , SO2 etc in Gdansk, Amsterdam and Odessa regions are presented. Our results can be considered as first examples of quite satisfactory short-range forecasts for the air pollutants.

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P80: New computational approach to the Earth atmosphere circulation and angle momentum balance modelling: Atmospheric circulation, teleconnection and radio-waveguides

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The satellite data and data of observing the radio-waveguide parameters (especially in the low troposphere layers) by means of radio-technical devices (in the ultra short-wave diapason) create the informative base of the modern atmosphere long-term forecasts. As any water quantities in atmosphere are formed on the basis of the cycle- and front-genesis (or in the convective non-stability lines) one can introduce the corresponding model on the basis of thermodynamics and hydro-mechanics of the corresponding processes. For example, physics of these processes can coincide with a soliton mechanics, which has the long-periodical base of the energy support. The action mechanics of such a soliton defines the key thermo-hydro-dynamical parameters of the atmospheric ultra-short-wave radio-waveguide. We present principally new methods of monitoring the Earth system low-frequency scale processes on the basis of observing some summated contributions of low frequency oscillations for geophysical factors. They base on the energy and angle moment balance relations and new scheme for calculation of the macro-turbulence regime in typical atmospheric processes, which are known as atmospheric circulation forms [1,2]. The balance analysis allows to predict the large-scaled atmospheric transformations and teleconnection phenomena and to give their quantitative description. We carried out a series of the computer experiments at the Pacific ocean region in order to study global mechanisms in the atmospheric models and check the seasonal sequences of the conservation (or disbalance) of the Earth atmosphere angle momentum and to provide new predictors for the long-termed and super long-termed forecasts of the low frequency atmospheric processes. The current function (complex velocity) fields are calculated for typical atmospheric circulation's forms. The experiments allowed quantitatively defining a direct link between an atmospheric turnover and atmospheric circulation forms through the front divider position and typical low frequency process of conservation of the angle moment balance. Besides, we have adapted the modified theory of the macro-turbulence for possible using the atmosphere radio-waveguides as a special effective predictors in the long-termed plan.

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P81: Distribution of barchan dunes using a lattice model

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Sand dunes are found in many places such as deserts, the sea bottom and the surface of Mars. They are formed through interplay between sand and air flow or water flow. When a strong flow blows, sand grains are dislodged from the sand surface. The entrained sand grains collide with the ground and are sometimes deposited. This process takes place repeatedly, resulting in the formation of a dune. The profile of the wind flow is modified by dune topography. Most fascinated dune is barchan, which is crescent dune. We reproduced many barchans in numerical simulations and investigate the dynamics.

The motion of sand grains is realized by two processes: saltation and avalanche. Saltation is the transportation process of sand grains by flow. The saltation length and saltation mass are denoted L and q, respectively. Saltation occurs only for cells on the upwind face of dunes. The saltation length L and the amount of transported sand q are modeled by the following rules,L = a+bh(x,y,t)-ch2(x,y,t), where a=1.0, b=1.0, and c=0.01 are phenomenological parameters. The last term is introduced for L not to become too large. Note that L is used only in the range where L increases as a function of h(x,y,t). The saltation mass is fixed at 0.1 for simplicity. In the avalanche process the sand grains slide down along the locally steepest slope until the slope relaxes to be (or be lower than) the angle of repose which is set to be 34○

We reproduced a few hundred of barchans in numerical field by above model. Barchan releases sand from tips of two horns. The downwind barchan can capture the sand stream. Also, barchans sometimes collide each other. These direct and indirect interaction forms complex barchan fields. The size distribution of a few thousand of barchans is fitted by lognormal distribution well. This indicated that the small barchans exist around the large ones and the large barchans are around small barchans. The average size of barchans increase as the amount of supplied sand do. Next, when two barchan corridors collide, the size of barchan in the boundary between corridors has two type. Type (I) is not decoupling distribution, which shows superposition of each distribution. Type (II) is a distribution of uniform size. Through collision and inter-dune sand stream, the size of each barchan become uniform.

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P82: A Mathematical Model for Solar and Anthropogenic Forcing of Global Climate

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Several complicated non-linear models exist which model the physical processes leading to global climate fluctuations. Some of the more advanced models use observed data to constrain various parameters involved. However, the exact processes that affect the globally averaged temperature variations are not well understood completely. We develop a physically motivated reduced climate model utilizing a novel mathematical formulation involving non-linear delay differential equations to study temperature fluctuations when subjected to an imposed solar radiative forcing. This study may provide pathways for understanding the response of the global climate to a combination of relevant, external and internal factors. We have further incorporated simplified equations to test the effect of speculated mechanisms of climate forcing and evaluated the extent of their influence. The findings are significant in our efforts to predict climate change and help in policy framing necessary to tackle it. Remarks:- We stress on areas identified as 'Low Levels of Scientific Understanding' by the IPCC 2007 and try to assess some widely debated concepts. The results obtained using this simple formulation have shown high degree of correlation with observations.

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P83: Direct simulation of outdoor blast waves

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In this poster we present a three years long work around an outdoor pyrotechnic site. Acoustic pressure signals were recorded from the near field (_~ 300 m) to the intermediate field (_~ 4000 m) for several azimuths. Highly resolved direct simulations (Euler equations with a detonation model, topography, vegetation, and detailed meteorological conditions) are shown to reproduce the signature of the signals. To save computational time, the coupling between this full nonlinear model with a simpler linear acoustic model is shown efficient. This tool is used to perform parametric studies to determine the most defavorable meteorological conditions for an acoustic anoyance point of view.

*Speaker

P84: Complex approach to the formation of ideas about the phenomenon of dynamic chaos for university students

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One of the most famous and potentially useful nonlinear dynamic effects is a bounded, chaotic behavior called chaos or deterministic noise.
Deterministic or dynamic chaos is a non-periodic oscillation in nonlinear deterministic systems, showing a high sensitivity to the initial conditions [1-2]. From the very beginning of dynamic chaos formation as a scientific direction, a great interest was shown while studying this phenomenon in a wide range of applied problems such as physics, astronomy, radio electronics, telecommunications, biology, including neurodynamics, and even financial analysis. Studies of chaos have clarified and gave new impulses to the study of a whole series of issues of general physical and general scientific significance. These changes have caused a number of methodological problems that need to be addressed in the development of methodology for teaching modern concepts and phenomena. The purpose of this article is to substantiate the methodology of teaching dynamic chaos in teaching physics, astronomy, electronics and related subjects in university. Initially, it is important to carefully select the material and adapt it to achieve a combination of scientific character and accessibility for students.

This report presents methodical methods of teaching dynamic chaos on the basis of authors' experience. The study of phenomenon of dynamic chaos can be carried out in four stages. The report presents the stages of studying the phenomenon within a 15-week course with a volume of 3 credits with lectures and laboratory works. The suggested methodology was tested at the Faculty of Physics and Technology of al-Farabi Kazakh National University for undergraduate students of the third year of specialty "Radio engineering, electronics and telecommunications" [3]. The lecture materials and computer laboratory works are continuously improved and updated every year. In our opinion, the proposed methodology makes it possible to achieve a better formation of students' knowledge of dynamic chaos, also to form the required skills and skills of working with nonlinear models of physics, and to develop practical skills in working with computer models.

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Author Index

Author Index