CECAM-Psik Research Conference

Multiscale Modeling from First Principles

Monday 9th, Morning: session 1

Multi-scale Materials

Chair : **Claudia Draxl**, Humboldt University

9.00 Introduction by the Chair

9.10 **Karsten Albe**, TU Darmstadt
Plastic Deformation of Nanocrystalline and Glassy Metal Alloys studied by a Hybrid Molecular Dynamics/Monte-Carlo Simulations

10.10 **Gus Hart**, Brigham Young University
Multiscale Alloy Modeling

11.00 Coffee Break

11.30 **Peter Kratzer**, Duisburg University
Multiscale Modeling of Au-catalysed GaAs nanowire growth

12.30 **Luca Ghiringilli**, FHI Berlin
Free Metal and Metal-oxide Clusters: beyond the Static, Monostructure Description

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Monday 9th, Afternoon: session 2

Thermodynamics, Statistical Mechanics, and Excited States from First Principles
Chair : **Matthieu Verstraete**, Liege University

16.30 Introduction by the Chair

16.40 **Jörg Neugebauer**, MPG Düsseldorf
Ab initio based Multiscale Modeling of Structural Materials: From a Predictive Thermodynamic Description to Tailored Mechanical Properties

17.30 Coffee Break

18.00 **Karsten Reuter**, TU Munich
Towards First-Principles Chemical Engineering

19.00 **Claudia Draxl**, Humboldt University
Exploring Electron-hole Pairs in Nanomaterials

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Tuesday 10th, Morning: session 3

Biological Systems and Neural Network Methods
Chair : **Matthias Rupp**, Basel University

9.00 Introduction by the Chair

9.10 **Ray Kapral**, University of Toronto
Molecular Machines and Self-propelled Nano-motors

10.00 **Paolo Carloni**, Jülich
Membrane Biophysics investigated by Multi-scale Methods

11.00 Coffee Break

11.30 **Jörg Behler**, Bochum University
Extending the Length and Time Scales of Atomistic Simulations Using Neural Network Potentials

12.30 **Christoph Dellago**, University of Vienna
Studying Nucleation Processes with Computer Simulations:
Neural Networks for Force Calculation and Structure Recognition

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Tuesday 10th, Afternoon. Poster session

P1 Francisco Alarcon *Lattice-Boltzmann method applied to micro-swimmer suspensions*

P2 Marta Dudek *Interplay between amikacin and its ribosomal binding site studied by molecular dynamics, spectroscopic, and calorimetric techniques*

P3 David Gao *Multiscale Modeling of NC-AFM Experiments*

P4 Vihar Georgiev *Molecular Metal-Oxide nanoelectronics*

P5 Henry Heitzer *First-Principles Calculation of Dielectric Response in Molecule-Based Materials*

P6 Thomas Heinemann *Multiscale modeling approach towards understanding coronene self-assembly*

P7 Nicola Kleppmann *Simulation of C60 non-equilibrium surface growth*

P8 Martin Lisal *DPD Simulations with Chemical Reactions: Application to Thermal Decomposition of RDX*

P9 Gaëtan Maurel *Toward the understanding of the polymer-filler interaction by using a multi-scale modeling*

P10 David Mebane *A Bayesian Framework for Uncertainty Quantification in Multi-Scale Models of Chemical Process Systems*

P11 Carlo Motta *Multi-scale method for charge transport in organic semiconductors*

P12 Karol Palczynski *Exploring molecular-scale crystal structure formation of para-Sexiphenyl by all-atom Molecular Dynamics computer simulations*

P13 Peter Palenčár *Thermal stability and self-assembly of long Ì±-helices in the gas phase*

P14 Sumathy Raman *ReaxFF, Parallel Replica Dynamics*

P15 Juliusz Stasiewicz *Fragment-Orbital Modeling of Charge Transport in RNA*

P16 Ralf Tonner *Adsorption on the semiconductor surfaces Si(001) and TiO2(110): prototypical cases for dispersion-corrected DFT methods*

P17 Ekaterina Voronina *Multiscale Simulation of Atomic Oxygen Impact on Nanostructures*

P18 Tongyu Wang *Multi-scale Modeling*

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Multiscale Modeling from First Principles

Wednesday11th, Morning: session 4

Stochastic Methods, Nonequilibrium States
Chair : **Christoph Dellago**, University of Vienna

9.00 Introduction by the Chair

9.10 **Ron Elber**, UT Austin
From Atomically Detailed Trajectories to Equations for the Density: Coarse graining by Milestoning

10.00 **Carsten Hartmann**, FU Berlin
Tackling Long Timescales in Molecular Dynamics

11.00 Coffee Break

11.30 **Giovanni Ciccotti**, La Sapienza University
Time-dependent Non-equilibrium Molecular Dynamics

12.30 **Pep Español**, UNED Madrid
Statistical Mechanics of Hamiltonian AdResS Adaptive Resolution Simulations

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Multiscale Modeling from First Principles

Wednesday 11th, Afternoon: session 5

Quantum Modeling
Chair : **Matthias Scheffler**

16.00 Introduction by the Chair

16.10 **Ali Alavi**, Cambridge University
Quantum Monte Carlo approach to Quantum Chemical Problems

17.00 Coffee Break

17.30 **Emilio Artacho**, Cambridge University and University of the Basque Country
Electronic Effects in Radiation Damage

18.30 **Alberto Castro**, University of Zaragoza
From the Femto- to the Atto-second Time Scale: Analysis and Control of the Electronic Motion with Time-dependent Density Functional Theory.

Dinner at 20.30 as usual

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Multiscale Modeling from First Principles

Thursday 12th,Morning: session 6 and Afternoon: excursion to Dali museum

Multi-scale in Complex Fluids

Chair : **Friederike Schmid**, Mainz University

9.00 Introduction by the Chair

9.10 **Ignacio Pagonabarraga**, University of Barcelona
Hybrid Kinetic Schemes for Modeling Complex Fluids

10.05 **Gerhard Gompper**, Jülich
Mesoscale Modeling of Blood Flow: From Single Cells to Blood Rheology

11.00 Coffee Break

11.30 **Dominic Tildesley**, CECAM, EPFL
The Friction between Structured Surfaces

12.30 **Kurt Kremer**, MPG Mainz
Adaptive Resolution Simulations for Soft Matter: Applications and New Developments
Many-body dissipative particle dynamics: application to realistic liquid mixtures

Lunch at 13.30, Bus for excursion leaves at 15.00 and conference dinner at 21.00 pm

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Friday 13th, Morning: session 7

Multi-scale in Complex Fluids (2)
Chair : **Michel Mareschal**, Zcam

9.00 **Modesto Orozco**, Barcelona
The Multi-Scale nature of DNA

10.00 **Dominic Tildesley**, CECAM
Concluding Remarks

10.30 Coffee Break

11.00 Bus number 1
16.00 Bus number 2

Saturday 14th, Bus 3 will leave at 10.00 am