27th Max Born Symposium on Multiscale Modeling of Real Materials

Program

Friday, September 17

16:00-18:00 Registration

Saturday, September 18

8:30-9:00 Registration

9:00-9:10 Opening.
Robert Olkiewicz, Dean of the Faculty of Physics and Astronomy

Session I

9:10-9:55 Peter Kratzer (Duisburg, Germany)
First-principles simulations of half-metallic Heusler alloys for tunneling magnetoresistance devices

9:55-10:40 Valeri Stepanyuk (Halle, Germany)
Spin-dependent effects in atomic-scale nanostructures

10:40-11:10 Coffee & tea break

Session II

11:10-11:55 Angelos Michaelides (London, UK)
Electronic structure simulations of water solid interfaces

11:55-12:15 Nikolay Negulyaev (Halle, Germany)
Self-ordering of Adatoms Promoted by Electronic Substrate-Mediated Interaction

12:20-14:00 Lunch.

Session III

14:00 -14:45 Danny Perez (Los Alamos, USA)
Recent developments and applications in accelerated molecular dynamics

14:45-15:30 Kristen Fichthorn (University Park, USA)
Controlling Kinetic Self-Assembly in Al(110) Homoepitaxy

15:30-15:50 Mahdi Shirazi (Cork, Ireland)
Multi-scale simulation of Atomic Layer Deposition

15:50-16:20 Coffee & tea break

Session IV

16:20-17:05 Marian Krajci (Bratislava, Slovak Republic)
Quasicrystals Investigated Using Density-Functional Methods: Bulk, Surface and Thin Films

17:05-17:25 Elwira Wachowicz (Wroclaw, Poland)
Effect of impurities on structural, cohesive, and magnetic properties of grain boundaries in α-Fe

17:25-17:45 Mirosław Kozłowski (Krakow, Poland)
Vacancy thermodynamics and diffusion-controlled processes in intermetallics for functional and construction material technologies

19:00 Conference Dinner

Sunday, September 19

Session V

9:00-09:45 Ted Einstein (College Park, Maryland, USA)
Distinctive Features in Growth on Vicinal Cu(100): Understanding the Role of Impurities by Calculating Key Energies and Simulating Morphology

9:45-10:30 Talat S. Rahman (Orlando, USA)
Self Learning Kinetic Monte Carlo Method and its application to cluster diffusion and island coarsening

10:30-11:00 Coffee & tea break

Session VI

11:00-11:45 Matti Alatalo (Lappeenranta, Finland)
Structural, electronic and optical properties of TiO_2 nanoparticles

11:45-12:05 Pawel Scharoch (Wroclaw, Poland)
Thermal properties from first principles with the use of the Free Energy Surface concept

12:05-12:25 Urszula D. Wdowik (Krakow, Poland)
Lattice dynamics of Co-deficient and Fe-doped CoO

12:25-14:00 Lunch.

Session VII

14:00-14:45 Matthias Scheffler (Berlin, Germany)
Role of van der Waals Interactions in Physics, Chemistry, and Biology

14:45 -15:30 John P. Perdew (New Orleans, USA)
Improved Meta-Generalized Gradient Approximation for Exchange and Correlation in Atoms, Molecules, and Solids

15:30-16:00 Coffee & tea break

Session VIII

16:00-16:45 Jacek A. Majewski (Warsaw, Poland)
Functionalization of carbon nanotubes - a key to nanotechnology?

16:45-17:05 David Holec (Leoben, Austria)
Surface energy of carbon fullerenes and nanotubes

17:05-17:25 Eduardo Machady-Chary (Grenoble, France)
Growth and self-organization of nanostructures using BART(BigDFT-ART nouvea).

17:25-18:30 Poster session, snacks & beverages.

Monday, September 20

Session IX

9:00-09:45 Karsten Reuter (Munich, Germany)
Beat the heat

9:45-10:30 Graeme Henkelman (Austin, USA)
Modeling core/shell and alloy nanoparticles for oxygen reduction

10:30-11:00 Coffee & tea break

Session X

11:00-11:45 Timo Jacob (Ulm, Germany)
Modeling Electrochemical Systems

11:45-12:05 Gerard Novell-Leruth (Tarragona, Spain)
Mechanism of HCl oxidation (Deacon process) over RuO_2

12:05-12:25 Tomasz Ossowski (Wroclaw, Poland)
Structure and stability of grain boundaries in iron

12:25-14:00 Lunch.