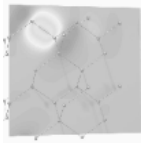
From Electrons to Phase Transitions

Vienna, February 26th to 28th 2014



Program and abstracts

Wednesday, February 26th 2014

08:30 – 09:00	***Registration***

Time	*Speaker*	*Title of Presentation*
09:00 – 09:10	***Welcome Words***	
09:10 – 09:45	E.K.U. Gross	Towards an ab-initio theory of superconductivity
09:45 – 10:20	Garnet Chan	How far are we from an ab-initio description of high Tc superconductivity?
10:20 – 10:50	***Coffee Break/Registration***	
10:50 – 11:25	Weitao Yang	Exchange-Correlation Energies and Electronic Excitation Energies from Pairing Matrix Fluctuations
11:25 – 11:45	Florian Libisch	Tackling Molecule-Surface Interactions Using Embedding Methods
11:45 – 12:05	Ferenc Karsai	Ab-initio study of the F Center in Lithium Fluoride
12:05 – 12:25	Joost VandeVondele	First-principles determination of the order-disorder phase transition in ordinary water ice
12:25 – 14:10	***Lunch Break***	
14:10 – 14:45	Ulrike Diebold	Back to Reality: Surfaces Investigated with STM and Spectroscopic Techniques
14:45 – 15:20	Claudine Noguera	Conditions of occurrence of metal-insulator transitions at polar-polar interfaces
15:20 – 15:40	Silvia Gallego	The surface Verwey transition at Fe3O4(001): emergence of surface polarons
15:40 – 16:00	Markus Aichhorn	Interplay of Hunds coupling, lattice coupling, and magnetism in oxide materials
16:00 – 16:30	***Coffee Break***	
16:30 – 17:05	Fakher Assaad	Quantum phase transitions in the Kane-Mele Hubbard model
17:05 – 17:25	Alessandro Toschi	Quantum many-body theory at the two-particle level: The new frontier
17:25 – 17:45	Sabine Andergassen	Correlations on all length scales by combining the DMFT and functional RG
17:45 – 18:05	Andreas Grüneis	Towards chemical accuracy in computational materials science

19:00 – 23:00	***Conference Dinner***

Thursday, February 27th 2014

Time	***Speaker***	***Title of Presentation***
09:00 – 09:35	Pieter Visscher	Rate Theory in Magnetic Materials
09:35 – 10:10	Roy Chantrell	Multiscale approaches to ultrafast phase transitions in magnetic thin films
10:10 – 10:40	***Coffee Break***	
10:40 – 11:15	Athanassios Z. Panagiotopoulos	Stabilizing Colloidal Crystal Phases by Leveraging Void Distributions
11:15 – 11:50	Friederike Schmid	New perspectives for molecular field simulations of complex fluids
11:50 – 12:10	Ulf R. Pedersen	Predicting crystals of metallic elements from the liquid state
12:10 – 12:30	Michael Grünwald	Driving self-assembly with simple external forces
12:30 – 14:10	***Lunch Break***	
14:10 – 14:45	Lucia Reining	A direct approach to the calculation of many-body Green's functions: beyond quasiparticles
14:45 – 15:20	David Singh	Discovery of New and Old Thermoelectrics using First Principles Methods
15:20 – 15:40	Miguel Martinez-Canales	Evolution of First-Row Elements at Multi-TPa Pressures
15:40 – 16:00	Martin Zelený	Ab initio study of Co- and Cu-doped Ni-Mn-Ga alloys
16:00 – 18:00	***Coffee Break & Poster Presentations***	

Friday, February 28th 2014

Time	***Speaker***	***Title of Presentation***
09:00 – 09:35	Olle Erikssen	Ab-initio spin-dynamics simulations; from electronic structure to marching skyrmions
09:35 – 09:55	Igor Abrikosov	Lattice vibrations, magnetic disorder, and their coupling at finite temperature
09:55 – 10:30	Frédéric Soisson	Atomistic simulations of diffusive phase transformations in iron-chromium alloys
10:30 – 10:50	Vsevolod Razumovsky	Spin-wave method for the total energy of paramagnetic state: application to iron and steel.
10:50 – 11:20	***Coffee Break***	
11:20 – 11:55	Anders Sandvik	Quantum Monte Carlo simulations of deconfined quantum-criticality
11:55 – 12:30	Lode Pollet	Dynamical correlation functions of U(1) critical models in (2+1) dimensions: can string theory help?
12:30 – 12:50	Andrej Gendiar	Mean-field universality induced by hyperbolic lattice curvature
12:50 – 13:00	***Farewell words***	