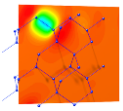


Wednesday, April 4th 2018

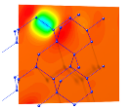
09:30 – 10:30	*Coffee Break / Registration (60 min)*

10:30 – 10:40	*Welcome Words*

Time	*Speaker*	*Title of Presentation*
10:40 – 11:20	Georg Madsen	Phonon superscatterers
11:20 – 12:00	Peter Blaha	Effects of different Exchange-Correlation approximations on various materials properties
12:00 – 12:20	Martin Panholzer	Optimized correlations: A practical pair density functional approach
12:20 – 14:00	*Lunch Break (1h 40 min)*	
14:00 – 14:40	Christoph Dellago	From electrons to phase transitions with neural networks: the case of water
14:40 – 15:20	Ignacio Pagonabarraga	Phase transitions and self assembly in active matter
15:20 – 15:40	Bengqing Cheng	Bridging the gap between atomistic and macroscopic models of homogeneous nucleation
15:40 – 16:10	*Coffee Break (30 min)*	
16:10 – 16:50	Tim Wehling	Electronic Correlations and Phase Transitions in Two-Dimensional Materials
16:50 – 17:30	Georg Kresse	Random phase approximation for materials modelling: melting point of Si
17:30 – 17:50	Kurt Lejaeghere	Modelling phase transitions in temperature-responsive flexible metal-organic frameworks: the delicate balance between dispersion and entropy

17:50 – 18:30	*Poster installation*

18:20 – 19:20	*Museum Albertina for invited speakers*
19:50 – 23:00	*Dinner for invited speakers*



Thursday, April 5th 2018

Time	*Speaker*	*Title of Presentation*
09:00 – 09:40	Carsten Honerkamp	Functional renormalization group for effective low-energy interactions
09:40 – 10:20	Karsten Held	Dynamical vertex approximation: a route to non-local electronic correlations
10:20 – 10:50	*Coffee Break (30 min)*	
10:50 – 11:30	Walter Metzner	Competition between magnetism and superconductivity in the Hubbard model and in the cuprates
11:30 – 12:10	Martin Eckstein	Photo-induced phases in Mott insulators
12:10 – 12:30	Irakli Titvinidze	Non-equilibrium real-space DMFT for correlated heterostuctures with long-range Coulomb interaction
12:30 – 14:10	*Lunch Break (1 h 40 min)*	
14:10 – 14:50	Maria Clelia Righi	*Ab initio* investigation of atomistic mechanisms in solid and boundary lubrication
14:50 – 15:10	Moritz to Baben	Bridging the gap from ab initio data to CalPhaD databases
15:10 – 15:30	Marco Arrigoni	First-principles calculations of harmonic force constants in random semiconductor alloys: effects on the prediction of the miscibility gap and thermal conductivity
15:30 – 16:10	Christos Likos	Liquid-drop model of soft nanocolloids: phase behavior beyond pairwise additivity
16:10 – 16:30	David Toneian	Dynamics of Magnetic Star Polymers
16:30 – 18:30	*Coffee Break & Poster Presentations*	

19:00 – 23:55	*Conference Dinner - Heuriger*

Friday, April 6th 2018

Time	*Speaker*	*Title of Presentation*
09:00 – 09:40	Michele Parrinello	Fluctuations, entropy and rare events
09:40 – 10:20	Jörg Neugebauer	From electrons to the design of structurally complex materials
10:20 – 10:40	Eduardo Hernandez	Thermodynamics of mantle minerals from first principles
10:40 – 11:00	Mojmir Sob	Phase stability in Fe, Co and Ni under High Strains and Surface Phase Transitions in Overlayers
11:00 – 11:30	*Coffee Break (30 min)*	
11:30 – 12:10	Ulrich Nowak	Simulating skyrmions in thin film multilayers
12:10 – 12:50	Dieter Suess	Heat-assisted magnetic recording – recent progress and future perspectives of multiscale modeling
12:50 – 13:00	*Farewell words*	