


ViCoM WORKSHOP OCTOBER 2011 / Schedule

03.10.2011 – 04.10.2011

Vers 2011_09_29

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SCHEDULE

Monday, 3. October 2011			
Time	Talk	Lecturers	Details
08:00 – 10:00	Bus Ride (Registered Passengers Only): Vienna – Stadtschlaining (120 min.)		
10:00 – 10:25	Check-In (25 min.)		
10:25 – 10:30	Hotel / Lounge → Conference Hall (5 min.)		
10:30 – 11:00	Coffee Break (Buffet, 30 min.)		
11:00 – 11:10	Greetings	Georg Kresse	Introductions etc.
11:10 – 11:50	Correlation effects in transport through quantum dots: renormalization-group approaches	Sabine Andergassen	Guest Lecture (35 min.) & Discussion (5 min.)
11:50 – 12:20	Towards million atoms: Semi-empirical potentials and inner eigenvalue solvers	Martijn Marsman	P02 Talk (25 min.) & Discussion (5 min.)
12:20 – 12:25	Conference Hall → Hotel / Dining Room (5 min.)		
12:25 – 13:55	Lunch (Buffet, 90 min.)		
13:55 – 14:00	Hotel / Dining Room → Conference Hall (5 min.)		
14:00 – 14:30	Optical conductivity with Wannier orbitals	Philipp Wissgott	P03 Talk (25 min.) & Discussion (5 min.)
14:30 – 15:00	Cluster update for Tensor Network States	Ling Wang	P04 Talk (25 min.) & Discussion (5 min.)
15:00 – 15:30	Coffee Break (Buffet, 30 min.)		
15:30 – 16:10	Stacking Fault Energies in Austenitic Steels from Density Functional Theory	Peter Puschnig	Guest Lecture (35 min.) & Discussion (5 min.)
16:10 – 16:40	Towards an accurate description of the electronic properties of graphene defect structures	Hasan Pašalić	P05 Talk (25 min.) & Discussion (5 min.)

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Monday, 3. October 2011 – Continuation			
Time	Talk	Lecturers	Details
16:40 – 17:10	Handling continua in time-dependent external fields	Armin Scrinzi	P06 Talk (25 min.) & Discussion (5 min.)
17:10 – 17:40	Calculation of NMR Chemical Shifts in APW based methods	Robert Laskowski	P07 Talk (25 min.) & Discussion (5 min.)
17:40 – 18:10	Spin order calculations for LaMnO₃ Quantum Monte Carlo - Stochastic Series expansion, application to NMR spectra.	Christoph Gruber Robert Achleitner	P09 Talks (2x 12 min.) & Discussion (5 min.)
18:10 – 18:15	Conference Hall → Hotel / Dining Room (5 min.)		
18:15 – 19:45*	Dinner (Buffet, 90 min.)		
19:25 – 19:30	ViCoM-Members Only: Hotel / Dining Room → Hotel / Meeting Room (5 min.)		
19:30 – 20:30	General Meeting (ViCoM-Members Only, 60 min.)		
End of Day 1			

*) 18:15 – 19:25 for ViCoM-Members

Tuesday, 4. October 2011			
Time	Talk	Lecturers	Details
07:30 – 08:30	Breakfast (Buffet, 60 min.)		
08:30 – 08:55	Check-Out (25 min.) – You may deposit your luggage at the hotel reception, but please do not forget that the accommodation facility does not assume any liability for lost or stolen valuables etc.		
08:55 – 09:00	Hotel → Conference Hall (5 min.)		
09:00 – 09:40	Multiscale computational tribology	Andras Vernes	Guest Lecture (35 min.) & Discussion (5 min.)
09:40 – 10:10	Progress Report on the Subproject P10: Cluster Expansion	Raimund Podloucky	P10 Talk (25 min.) & Discussion (5 min.)
10:10 – 10:40	Coffee Break (Buffet, 30 min.)		
10:40 – 11:20	Multi-scale modelling of high-temperature magnetization dynamics.	Oksana Chubykalo-Fesenko	Guest Lecture (35 min.) & Discussion (5 min.)
11:20 – 11:50	Accelerated Langevin simulations for calculating rare switching events using Forward Flux Sampling	Christoph Vogler	P12 Talk (25 min.) & Discussion (5 min.)
11:50 – 12:20	Factors contributing to the glass-forming ability of a simulated molecular liquid	Ulf Rørnbæk Pedersen	P11 Talk (25 min.) & Discussion (5 min.)
12:20 – 12:25	Conference Hall → Hotel / Dining Room (5 min.)		
12:25 – 13:55	Lunch (Buffet, 90 min.)		
13:55 – 14:00	Hotel / Dining Room → Conference Hall (5 min.)		
14:00 – 14:50	Discussion (Focus Groups, 50 min.)		
14:50 – 15:00	Farewell	Georg Kresse	Event Announcements etc.
15:00 – 15:15	Conference Hall → Hotel (Luggage) → Bus Stop (15 min.)		
15:15 – 17:50	Bus-Ride (Registered Passengers Only): Stadtschlaining – Stopover: Vienna Airport “Wien-Schwechat” (Arrival at 17:15) – Vienna (150 min.)		
End of Day 2, End of the Workshop			