



International Max Planck Research School

Dynamical Processes in Atoms, Molecules, and Solids

IMPRS Retreat 2012, Seminarhotel Frohberg, Sept. 25-27

Tue, Sept. 25th

12.00	Arrival
12.30-13.30	Lunch
13.30-13.45	WELCOME: Michael Genkin
13.45-14.00	Introduction of the participants

Partners Presentations I: (Chair: Michael Genkin)

14.00-14.25	Stefan Kirchner
14.25-14.50	Ulf Saalmann
14.50-15.15	Kathrin Padberg-Gehle
15.15-15.40	Matthias Vojta
15.40-16.10	Coffee

Partners Presentations II: (Chair: Ulf Saalmann)

16.10-16.35	Jan Michael Rost
16.35-17.00	Pavel Jungwirth
17.00-17.25	Frank Pollmann
18.00	Dinner
19.00	Social get-together

Wed., Sept. 26th

“Semiclassics & Molecular Dynamics I” (Chair: Lena Simon)

- 9.00-9.25 **Michael Fischer** (TUD)
Non-adiabatic quantum molecular dynamics with surface hopping
- 9.25-9.50 **Eva Pluharova** (IOCB)
Ion pairing of Li⁺ in water by classical and ab initio MD
- 9.50-10.15 **Carlos Zagoya** (MPIPKS)
A semi-classical approach to quantum breathers
- 10.15-10.45 Coffee

“Spins & Solids” (Chair: Fabian Maucher)

- 10.45-11.10 **Johannes Knolle** (MPIPKS)
Dynamical spin correlations in a quantum spin liquid
- 11.10-11.35 **Dorota Komornicka** (ILTSR)
The local structure of crystals - the use of differential evolution algorithm in modeling of diffuse scattering
- 11.35-12.00 **Salim Erfanifam** (HZDR)
Elastic properties of spin ices
- 12.15 Lunch
- 13.30 Hiking tour
- 18.00 Dinner

“Photoionization” (Chair: Laura Gil)

- 19.00-19.25 **Abraham Camacho** (MPIPKS)
Electron Spectra of Fullerene under Intense XFEL Pulses
- 19.25-19.50 **Ondrej Svoboda** (PICT)
Nonadiabatic photoionization dynamics of water dimer
- 19.50-20.15 **Elias Diesen** (MPIPKS)
Structures in low-energy spectra of photoelectrons from high-intensity laser fields
- 20.00 Social get-together

Thu., Oct. 27th

“Semiclassics & Molecular Dynamics II” (Chair: Thomas Brumme)

- 9.00-9.25 **Karsten Leonhardt** (MPIPKS)
Interplay of conical intersections and entanglement transport in two-dimensional flexible Rydberg aggregates
- 9.25-9.50 **Lena Simon** (TUD)
Semiclassical dynamics of ultracold bosons in multiple wells
- 9.50-10.15 **Max Buchholz** (TUD)
Semiclassical hybrid approach to the dynamics of iodine in solid krypton
- 10.15-10.45 Coffee

“Chemical Processes & Imaging” (Chair: Hugo Vieyra)

- 10.45-11.10 **Tim Ludwig** (TUD)
Master-equation approach for simulating STM images of single molecules
- 11.10-11.35 **Jana Paterova** (IOCB)
Molecular Mechanisms of Ion-Specific Effects on Proteins
- 11.35-12.00 **Daniele Selli** (TUD)
Structure prediction and modeling: quest for new materials
- 12.00-12.25 **Frank Uhlig** (IOCB)
Unraveling the complex nature of the hydrated electron
- 12.45 Lunch & Departure