

Transferability Issues in Multiscale Modeling of Hierarchical Phenomena

Hermann Staudinger Lecture Hall

Ackermannweg 10

55128 Mainz

Monday 7 December 2015

- 08:50 - 09:00 **Welcome: Friederike Schmid**
- 09:00 - 09:50 **Ard Louis (Oxford)**
No-free lunch theories for coarse-graining
- 09:50 - 10:40 **Ivan Coluzza (Vienna)**
*Transferable coarse-grained potential model
for quantitative protein folding and design*
- 10:40 - 11:10 **Coffee**
- 11:10 - 12:00 **Simón Poblete (SISSA)**
*Testing potentials beyond the parametrization:
Examples from protein dynamics and RNA structure*
- 12:00 - 12:30 **Tristan Beraud (MPIP)**
Automated force field parametrization across chemical space
- 12:30 - 14:30 **Lunch with Posters**
- 14:30 - 15:20 **Nico van der Vegt (Darmstadt)**
Transferability of free energy-based potentials
- 15:20 - 16:10 **Evangelia Kalligiannaki (Crete)**
*Coarse graining non-equilibrium systems
and path space information theory*
- 16:10 - 16:40 **Coffee**
- 16:40 - 17:30 **Cahit Dalgıçdir (Darmstadt)**
*A transferable coarse-grained model of diphenylalanine
for environment driven conformational transition*
- 17:30 - 18:00 **Joseph Rudzinski (MPIP)**
*Deriving transferable models for ionomer aggregation
using the generalized Yvon-Born-Green framework*
- 18:00 - 18:05 **Farewell**