

Complex High-Dimensional Energy Landscapes

Tuesday September 19, 2017

- 2:30–3:00 **Augustin Chevallier** (Université de Nice Sophia Antipolis)
Wang-Landau: adaptive random walk for fast convergence
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Joshua Paul** (University of Florida)
2D Material Characterization, Discovery, and Potential Machine Learning Applications

Thursday September 21, 2017

- 2:30–3:00 **Florent Hedin** (École des Ponts ParisTech)
The Generalized ParRep algorithm: developing an OpenMM based implementation for studying biochemical systems
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Justin Smith** (University of California, Los Angeles (UCLA))
Finding the right density from the wrong temperature with thermal density functional theory

Tuesday September 26, 2017

- 2:30–3:00 **Anne Marie Tan** (University of Illinois at Urbana-Champaign)
Computing the lattice Green function for dislocations in complex materials
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Marco Di Gennaro** (University of Basel)
The role of complexity in Quantum Machine Learning models for crystals

Thursday September 28, 2017

- 2:30–3:00 **Andreas Smolenko** (RWTH Aachen)
Computing the shadow Hamiltonian
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Biswas Rijal** (University of Florida)
The challenges in study of point defects in two dimensional materials



Tuesday October 10, 2017

- 2:30–3:00 **Laura Lopes** (École Nationale des Ponts-et-Chaussées (ENPC))
Application of the Adaptive Multilevel Splitting Method in Molecular Dynamics
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Wei Zhang** (Free University of Berlin and Zuse Institute Berlin)
Analysis of transition pathways for jump processes and connections with transition path theory

Thursday October 12, 2017

- 2:30–3:00 **Feliks Nüske** (Rice University)
Projection Formalism and Effective Dynamics for Stochastic Dynamics
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Mauricio del Razo Sarmina** (Freie Universität Berlin)
Coupling Markov state models of molecular kinetics with reaction-diffusion simulations

Tuesday October 24, 2017

- 2:30–3:00 **Pierre Terrier** (École Nationale des Ponts-et-Chaussées)
Cluster dynamics in materials: a hybrid deterministic/stochastic coupling algorithm
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Hao Wu** (Free University of Berlin and Zuse Institute Berlin)
Variational approach for Markov processes

Thursday October 26, 2017

- 2:30–3:00 **Zofia Trstanova** (University of Edinburgh)
Diffusion-map directed sampling
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Lorenzo Boninsegna** (Rice University)
Data-driven perspective on coarse graining modelling

Tuesday November 7, 2017

- 2:30–3:00 **Giovanni Pinamonti** (Freie Universität Berlin)
Modelling the unzipping of the neuronal SNARE complex
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Ting Wang** (University of Delaware)
Parallel replica dynamics for multi-scale Markov jump processes

Thursday November 9, 2017

- 2:30–3:00 **Jan Janssen** (Max-Planck-Institut für Eisenforschung GmbH)
Towards an Uncertainty Quantification for Ab Initio Thermodynamics
- 3:00–3:30 *Tea Time*
- 3:30–4:00 **Nestor Aguirre** (Los Alamos National Laboratory)
Statistical Simulation of Molecular Fragmentation Processes