

Energy Landscapes: Structure, Dynamics and Exploration Algorithms

(07/17/2017 - 07/21/2017)

Participants:

1. **Arts, Milou** (University of Amsterdam, milou.arts@student.uva.nl) :
Transition networks of biological systems
2. **Begay, Shanadeen** (Northeastern University Boston, scbegay@bu.edu) :
Thermodynamics and structure of biological molecules
3. **Buchete, Nicolae-Viorel** (University College Dublin, buchete@ucd.ie) :
Coarse master equations with replica exchange molecular dynamics
4. **Hoffmann, Karl Heinz** (Technische Universität Chemnitz, hoffmann@physik.tu-chemnitz.de) :
Statistical physics, Hidden Markov Models
5. **Jeanmairet, Guillaume** (Université Pierre et Marie Curie, guillaume.jeanmairet@upmc.fr):
Driven phase transition via molecular dynamics simulation for chemical systems
6. **Lazauskas, Tomas** (University College London, t.lazauskas@ucl.ac.uk) :
Structure prediction using a grand canonical approach
7. **Prehl, Janett** (Technische Universität Chemnitz, janett.prehl@physik.tu-chemnitz.de) :
Modelling twin polymerization
8. **Roach, Ty** (San Diego State University, smokinroachjr@gmail.com) :
Application of thermodynamics on biological systems
9. **Rosta, Edina** (Kings College London, edina.rosta@kcl.ac.uk) :
Method developments for finding the width of transition states
10. **Salamon, Peter** (San Diego State University, psalamon@mail.sdsu.edu) :
The Ladder-Theorem
11. **Schoen, Christian** (MPI for Solid State Research, c.schoen@fkf.mpg.de) :
Macroscopic vs. microscopic landscapes – development of the threshold algorithm
12. **Schwalbe, Karsten** (Technische Universität Chemnitz, karsten.schwalbe@physik.tu-chemnitz.de) :
Optimal control of stochastic processes
13. **Shehu, Amarda** (George Mason University, armada.shehu@gmail.com) :
Data-driven Stochastic Optimization for Sample-based Models of Protein Energy Landscapes
14. **Woodley, Scott M.** (University College London, scott.woodley@ucl.ac.uk) :
Temperature depending clustering – what energy with what temperature?

Time	Monday	Tuesday	Wednesday	Thursday	Friday
9:00	Organizational Meeting	Guillaume Jeanmairet	Edina Rosta	Tomas Lazauskas	Ty Roach
10:00	Christian Schön				Janett Prehl
11:00		Amarda Shehu	Shanadeen Begay	Milou Arts	
12:00	Nicolae-Viorel Buchete				Scott M. Woodley
14:00					Wrap-Up-Session