



Funded by **DFG**

Spring School 2016: Molecular Dynamics Program

Date: 25-29 April 2016

Venue: Burghotel Bad Belzig, Wittenbergerstr. 14, 14806 Bad Belzig,
www.burghotel-bad-belzig.de

Monday, 25.04.

10:00 - 11:00	Arrival and registration
11:00 - 12:00	Introduction (Bettina Keller, Petra Imhof, Carsten Hartmann, Marcus Weber)
12:00 - 13:30	LUNCH BREAK
13:30 - 15:30	Three perspectives on molecular dynamics: chemistry, physics, mathematics (Bettina Keller, Petra Imhof, Carsten Hartmann)
15:30 - 16:00	COFFEE BREAK
16:00 - 18:00	Root models for different types of dynamics (Carsten Hartmann)
18.00 - 19.00	DINNER
19.00 - 20.30	Getting to know each other: introducing each other's PhD projects

Tuesday, 26.04.

09:00 - 09:15	What is „entropy“?
09:15 - 10:15	Statistical mechanics I (Petra Imhof)
10:15 - 10:45	COFFEE BREAK
10:45 - 11:00	What is „an ensemble“?
11:00 - 12:00	Statistical mechanics II (Petra Imhof)
12:00 - 13:30	LUNCH BREAK
13:30 - 13:45	What is „energy function“?
13:45 - 14:45	Molecular dynamics simulations I (Bettina Keller)
14:45 - 15:15	COFFEE BREAK
15:15 - 15:30	What is „coarse graining“?
15:30 - 16:30	Molecular dynamics simulations II (Bettina Keller)
16:30 - 18:30	Freetime activity, e.g. walk in the town or in the nature, sports etc.
18:30 - 19:30	DINNER
Evening:	Freetime

Wednesday, 27.04.

09:00 - 09:15 What is „MCMC“?
09:15 - 10:15 Hybrid Monte Carlo / Symplecticity (Marcus Weber)
10:15 - 10:45 COFFEE BREAK
10:45 - 11:00 What is „spectral analysis“?
11:00 - 12:00 Transfer Operators (Marcus Weber)

12:00 - 13:30 LUNCH BREAK

13:30 - 14:45 Metastability / PCCA+ (Marcus Weber)
14:45 - 15:15 COFFEE BREAK
15:15 - 15:30 What is „Markovianity“?
15:30 - 16:30 Eigenfunctions / Committor Functions / Invariant Spaces (Marcus Weber)
16:30 - 17:00 COFFEE BREAK
17:00 - 18:30 Discretization Schemes / Applications (Marcus Weber)

18:30 - 19:30 DINNER
Evening: Freetime

Thursday, 28.04.

09:00 - 12:00 Group work: preparing a short proposal for a collaborative research project

12:00 - 13:30 LUNCH BREAK

13:30 - 13:45 What is „a nonequilibrium steady-state“?
13:45 - 15:45 Special guest: Gabriel Stoltz, CERMICS, École des Ponts ParisTech,
 topic: tba
15:45 - 16:15 COFFEE BREAK
16:15 - 16:30 What is „an open system“?
16:30 - 18:30 Special guest from the CRC 1114: Christof Schütte, topic: tba

18:30 - 19:30 DINNER

19:30 - 21.00 Presentation of the research proposals to the board of reviewers (instructors
 and special guests), prize-giving ceremony

Friday, 29.04.

09:30 - 10:15 Which research questions are raised within the SFB 1114 from a
 chemical, a physical, and a biological view point? (Bettina Keller)
10:15 - 10:45 COFFEE BREAK
10:45 - 11:30 Which mathematical tools are used within the SFB 1114 to solve
 these questions? (Carsten Hartmann)
11:30 - 12:30 LUNCH BREAK
12:30 - 14:00 Open forum
14.43 Departure by train from Bad Belzig railway station