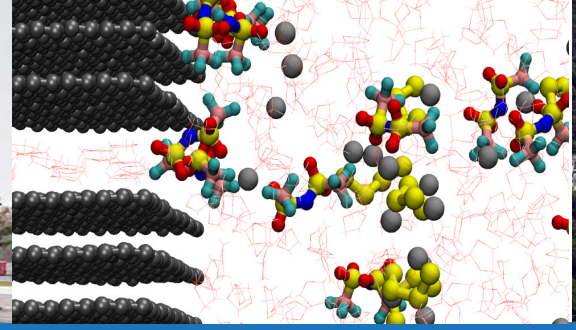


Workshop venue:

Lise-Meitner Campus, Hahn-Meitner-Platz 1, 14109 Berlin (Wannsee)
Room: "Kolloquiumsraum", H 132

Travel instructions:

***S+U Berlin Hbf (Central station)→ S Wannsee Bhf**

- S7 Direction: S Potsdam Hauptbahnhof
- RE1 Direction: Brandenburg, Hauptbahnhof
- RB21 Direction: Wustermark, Bahnhof

***S+U Zoologischer Garten→ S Wannsee Bhf**

- S7 Direction: S Potsdam Hauptbahnhof
- RE1 Direction: Brandenburg, Hauptbahnhof
- RB21 Direction: Wustermark, Bahnhof

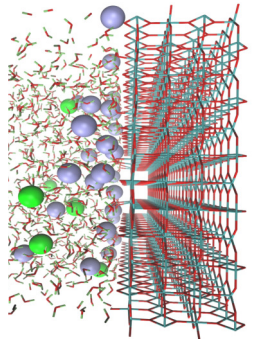
***S Wannsee Bhf → Hahn-Meitner-Platz 1**

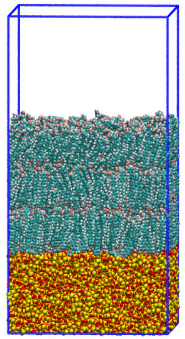
- Bus 318 Direction: Hahn-Meitner-Platz

An alternative connection:

- Bus 118 Direction: Drewitz, Stern-Center (exit: Wilhelmplatz)

2nd International workshop on the Multi-Scale Modeling of Functional Interfaces and Soft Materials

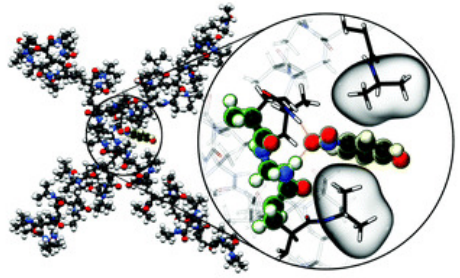


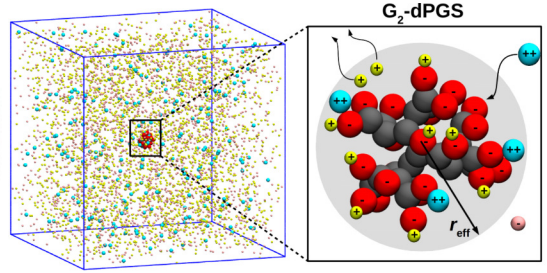


March 4 - 6, 2020

Helmholtz Zentrum Berlin

Berlin, Germany





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HUMBOLDT-UNIVERSITÄT ZU BERLIN

UNI FREIBURG

HZB Helmholtz Zentrum Berlin

Wed., March 4th 2020

- **14:00 – 14:15** *Joachim Dzubiella*
  Welcome word

Functional Polymers

- **14:15 – 14:45** *Jan Heyda*
- **14:45 – 15:15** *Gregor Richard Weiss*
- **15:15 – 15:45** *Simon Gramatte*

15:45 – 16:30 Coffee break

- **16:30 – 17:00** *Matej Kanduč*
- **17:00 – 17:30** *Won Kyu Kim*
- **17:30 – 18:00** *Sebastian Milster*

18:00 – 19:00 Dinner Cafe Jahn

- **19:00 – 19:30** *Stefano Angioletti-Uberti*
- **19:30 – 20:00** *Rohit Nikam*

Thurs., March 5th 2020

Solid-Liquid Interfaces

- **9:30 – 10:00** *Benjamin Rotenberg*
- **10:00 – 10:30** *Zhujie Li*
- **10:30 – 11:00** *Victor Ruiz*

11:00 – 11:45 Coffee break

- **11:45 – 12:15** *Sebastien Groh*
- **12:15 – 12:45** *Mila Miletic*
- **12:45 – 13:15** *Chanbum Park*

13:15 – 14:00 Lunch break

Reaction – Diffusion

- **14:00 – 14:30** *Rafael Roa*
- **14:30 – 15:00** *Michael Bley*
- **15:00 – 15:30** *Goh Kek Boon*

15:30 – 16:15 Coffee break

- **16:15 – 16:45** *Upayan Baul*
- **16:45 – 17:15** *Yi-Chen Lin*

19:00 – 23:00 Dinner Dogtap Brewdog

Fri., March 6th 2020

Molecules – Clusters – Spectroscopy

- **9:30 – 10:00** *Annika Bande*
- **10:00 – 10:30** *Fabian Weber*

10:30 – 11:15 Coffee break

- **11:15 – 11:45** *Caterina Cocchi*
- **11:45 – 12:15** *Holger Saßnick*
- **12:15 – 12:45** *Yannik Schütze*

12:45 Lunch break

End of Workshop

Session I (Wed. March 4th 2020): Functional Polymers

Time:	Name:	Title:
14:15 – 14:45	Jan Heyda	*Thermodynamic properties of single and many pNIPAM chains in aqueous solutions*
14:45 – 15:15	Gregor Richard Weiss	*Replacing the arbitrariness from `modeler's choices in Markov State Modeling by physically-based decision processes*
15:15 – 15:45	Simon Gramatte	*Computational Study of Structure and Dynamics of Polycarbonate Nanodroplets: Glass or Liquid?*
16:30 – 17:00	Matej Kanduč	*Permeability at the molecular scale*
17:00 – 17:30	Won Kyu Kim	*Effects of active solutes on the cosolute permeability in polymer networks*
17:30 – 18:00	Sebastian Milster	*The cross-linker effect on the permeability of regular polymer networks*
19:00 – 19:30	Stefano Angioletti-Uberti	*Theory and experiments in multivalent nanoparticles for targeted drug delivery: some recent results*
19:30 – 20:00	Rohit Nikam	*Competitive partitioning of mono- versus divalent ions in highly charged macromolecules*

Session II (Thurs. March 5th 2020): Solid-Liquid Interfaces

9:30 – 10:00	Benjamin Rotenberg	*Influence of electrode metallicity in molecular simulations: a semi-classical Thomas-Fermi model*
10:00 – 10:30	Zhujie Li	*Ion-specific Adsorption on Bare Gold Nanoparticles: Solvation Structure and Surface Potentials*
10:30 – 11:00	Victor Ruiz	*Atomistic modelling of complex interfaces: from theoretical surface science to solid-liquid interfaces*
11:45 – 12:15	Sebastien Groh	*From surface defects to EDL properties: Application to the TiO_2/electrolyte system*
12:15 – 12:45	Mila Miletic	*Influence of polarity on adsorption and growth of conjugated organic molecules on inorganic substrates*
12:45 – 13:15	Chanbum Park	*Li/S electrolytes on graphene interface*

Session III (Thurs. March 5th 2020): Reaction – Diffusion

14:00 – 14:30	Rafael Roa	*Degradation of enzyme-sensitive hydrogels*
14:30 – 15:00	Michael Bley	*Simulation of non-equilibrium reactions towards transient structures and polymer networks*
15:00 – 15:30	Goh Kek Boon	*Time-varying nanoreactors*
16:15 – 16:45	Upayan Baul	*Polydispersity as an adaptive response: computer simulations of soft particles*
16:45 – 17:15	Yi-Chen Lin	*Electrostatic inhibition induced by charged end-products*

Session IV (Fri. March 6th 2020): Molecules – Clusters – Spectroscopy

9:30 – 10:00	Annika Bande	*Zooming in on electrons: electronic structure and dynamics*
10:00 – 10:30	Fabian Weber	*Model Water-Splitting Dynamics at N-doped Graphene Oxides*
11:15 – 11:45	Caterina Cocchi	*Electronic and optical properties of (doped) organic semiconductors from ab initio many-body theory*
11:45 – 12:15	Holger Saßnick	*First-principles characterization of the adsorption properties of water on titanium dioxide surfaces*
12:15 – 12:45	Yannik Schütze	*First-principles study of thiophenyl benzenethiol as sulfur host material for Li/S batteries: relative stability upon reduction*