International Workshop
Molecular Modeling and Simulation in Applied Material Science

Organized in co-operation with

SPP 1155 DFG — Deutsche Forschungsgemeinschaft DFG — SFB 716 — ProcessNet, eine Initiative von DECHEMA und VDI-GVC

Programme
Monday, March 10, 2008

11:00 **Opening address**
H. Hasse, University of Stuttgart/D

Opening Session Day 1

Chair: H. Hasse, University of Stuttgart/D

11:05 **Applications of molecular simulation in energy- and environment-related research**
P. Ungerer, Institut Francais du Pétrole, Rueil-Malmaison/F

11:30 **Molecular simulations of amorphous polymers: meeting the challenge of long time scales**
D.N. Theodorou, National Technical University of Athens/GR

11:55 **Magnetic tight binding theory: application to the heat of mixing of dilute iron-chromium alloys**
A.T. Paxton, M.W. Finnis, Queen's University Belfast/UK

12:20 Lunch break

Polymers

Chair: J. Vorholz, Evonik Röhm GmbH, Darmstadt/D

13:30 **Multiscale modelling of polymers: useful for problems in industry**
F. Müller-Plathe, Technical University of Darmstadt/D

13:50 **On polyethylene cable failure, electric fields, water clusters and ions**
E. Johansson, K. Bolton, P. Ahlström, University College of Borås/S

14:10 **Controlling wettability and flow at surfaces by polymer coatings**
M. Müller, C. Servantie, University of Göttingen/D; C. Pastorino, CNEA-CONICET, Buenos Aires/RA

14:30 **Water bridging and clustering in amorphous Kapton®: a molecular dynamics simulation study**
S. Neyertz, G. Marque, University of Savoie, Bourget du Lac/F; J. Verdu, ENSAM, Paris/F; V. Prunier, EDF, Moret-sur-Loing/F; D. Brown, University of Savoie, Bourget du Lac/F

14:50 **Structure and dynamics of entangled polystyrene melts using coarse-graining MD simulations**
V. Harmandaris, N. van der Vegt, K. Kremer, MPI for Polymer Research, Mainz/D

15:10 Coffee break

Industrial Fluids (Parallel Session)

Chair: S. Schmauder, University of Stuttgart/D

15:40 **MD investigation of the formation of zinc nanoparticles**
S. Braun, F. Römer, T. Kraska, University of Cologne/D

16:00 **Model of adsorption processes at the glass surface in the presence of oxalic acid**
J. Kundin, C.-J. Yu, H. Emmerich, RWTH Aachen University/D

16:20 **Modeling of unit operations by molecular simulations**
D. Babic, A. Pfennig, RWTH Aachen University/D

16:40 **Formation and pyrolysis of polymethylsilsesquioxane using quantum-chemical methods**
L. Rutz, H. Bockhorn, University of Karlsruhe/D

17:00 Coffee break

Diffusion (Parallel Session)

Chair: C. Elsässer, FhI for Mechanics of Materials, Freiburg/D

15:40 **Diffusion through heterogeneous nanochannels: a first-passage time approach**
A.J. Dammers, V.J. van Hijkoop, M.-O. Coppens, Delft University of Technology/NL

16:00 **Diffusion of hydrocarbon mixture in one-dimensional zeolite channel**
S. Chatterjee, G.M. Schuetz, Research Centre Juelich GmbH/D

16:20 **Simulation and analytical treatment of the mass-transfer through zeolite surfaces for the ad- and desorption of molecules**
A. Schüring, University of Leipzig/D; J. Gulín-González, University of Informatics Science, Havanna/C; S. Vasenkov, University of Florida, Gainesville, FL/USA; S. Fritzsche, J. Kärger, University of Leipzig/D

16:40 **In-depth study of the influence of host-framework flexibility on the diffusion of small gas molecules in zeolitic pore systems**
N. Zimmermann, S. Jakobtorweihen, University of Technology, Hamburg/D; B. Smit, CECAM, Lyon/F; F.J. Keil, University of Technology, Hamburg/D

17:00 Coffee break

Crystalline Materials

Chair: F.J. Keil, University of Technology, Hamburg/D

17:30 **Ab-initio modeling of materials for heterogeneous catalysis**
B. Meyer, University of Erlangen-Nuremberg/D

17:50 **Ab-initio thermodynamics of metallic alloys and compounds**
S. Müller, University of Erlangen-Nuremberg/D

18:10 **Optimizing materials properties and epitaxial growth of semiconductor devices by ab initio based multiscale modeling**
J. Neugebauer, MPI for Iron Research GmbH, Düsseldorf/D

18:30 **First-principles modelling of interface-controlled properties of insulating and conducting materials for integrated functional devices**
C. Elsässer, FhI for Mechanics of Materials, Freiburg/D

18:50 **Computer simulations from atoms to components**
S. Schmauder, University of Stuttgart/D

19:10 **Understanding complexity in intermetallic alloys**
H.-R. Trebin, M. Engel, University of Stuttgart/D

19:30 Get-together in a traditional Frankfurt cider tavern

Tuesday, March 11, 2008

Opening Session Day 2

Chair: F. Müller-Plathe, Technical University of Darmstadt/D

08:00 **Ab-initio force field and thermodynamic properties**
H. Sun, Shanghai Jiao Tong University/PRC

08:25 **Molecular design of rubbery polymers for membrane applications**
I.G. Economou, Z. Makrodimitri, National Research Center for Physical Sciences "Demokritos", Agia Paraskevi Attikis/GR

08:50 **Directed assembly of block copolymers and its application for nano-fabrication**
J.J. de Pablo, University of Wisconsin, Madison, WI/USA

09:15 Coffee break

Industrial Applications

Chair: J. Vrabec, University of Stuttgart/D

09:45 **Predictive molecular modeling: Monte Carlo meets equations of state**
F. Heilmann, G. Fernandez, M. Heilig, B. Banaszak, BASF SE, Ludwigshafen/D

10:05 **Simulation at various spatial and temporal scales in process technology**
J. Vorholz, Evonik Röhm GmbH, Darmstadt/D

10:25 **Computational materials science for industrial R&D**
A. Mavromaras, Materials Design, Årsta/S; E. Wimmer, Materials Design, Le Mans/F

10:45 **COSMOtherm: thermophysical data of liquid systems from ab-initio quantum chemistry**
A. Klamt, COSMOlogic GmbH & Co. KG, Leverkusen/D

11:05 **Unravelling the interaction of ammonia with carbon nanotubes**
G. Goldbeck-Wood, C. Oliva, P. Strodel, Accelrys, Cambridge/UK; A. Maiti, Lawrence Livermore National Laboratory, CA/USA

11:25 **Multiscale simulations of green solvents : from ab initio to physical properties modeling**
A. Bick, X. Krokidis, L. Peristeras, Scienomics GmbH, Ottobrunn/D;
I.G. Economou, National Research Center for Physical Sciences "Demokritos", Agia Paraskevi Attikis/GR

11:35 Coffee break

Methods

Chair: H.R. Trebin, University of Stuttgart/D

11:55 **Complex systems with many-body interactions: efficient multi-particle move sampling in Monte Carlo simulations**
I. Nezbeda, J.E. Purkinje University, Usti nad Labem/CZ

12:15 **Molecular modeling approaches for calculating excess chemical potentials of large-size molecules in polymeric microstructures**
B. Hess, T.A. Ozal, C. Peter, N.F.A. van der Vegt, MPI for Polymer Research, Mainz/D

12:35 **High performance computing aspects of molecular simulations**
H.J. Bungartz, Technical University of Munich/D

12:55 **Visualization of molecular simulations**
D. Weiskopf, University of Stuttgart/D

13:15 Lunch break

Closing Session

Chair: H. Hasse, University of Stuttgart/D

14:15 **Molecular simulation of the synthesis of periodic mesoporous silica materials**
M. Jorge, University of Porto/P; N.A. Seaton, University of Edinburgh/UK

14:35 **On the application of force fields for predicting a wide variety of properties: ethylene oxide as an example**
J. Vrabec, B. Eckl, H. Hasse, University of Stuttgart/D

14:55 **Activity coefficients of associating fluids in aqueous solution by molecular dynamics simulation**
J. Fischer, J. Caßens, D. Paschek, G. Sadowski, Technical University of Dortmund/D

15:15 **Adsorption from dilute solutions: the mean force method**
J. Fischer, R. Tscheliessnig, W. Billes, M. Wendland, University of Vienna/A

15:35 **Polymer and monomer adsorption on anhydrite or gypsum surfaces**
S. Fritz, W. Voigt, Technical University Bergakademie Freiberg/D

15:55 **Multiscale modeling of human skin**
G. Goldbeck-Wood, R. Akkermans, Accelrys, Cambridge/UK

16:15 Closing remarks and end of the workshop

Conference office and venue:

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