DECHEMA
Gesellschaft für Chemische Technik
und Biotechnologie e.V.

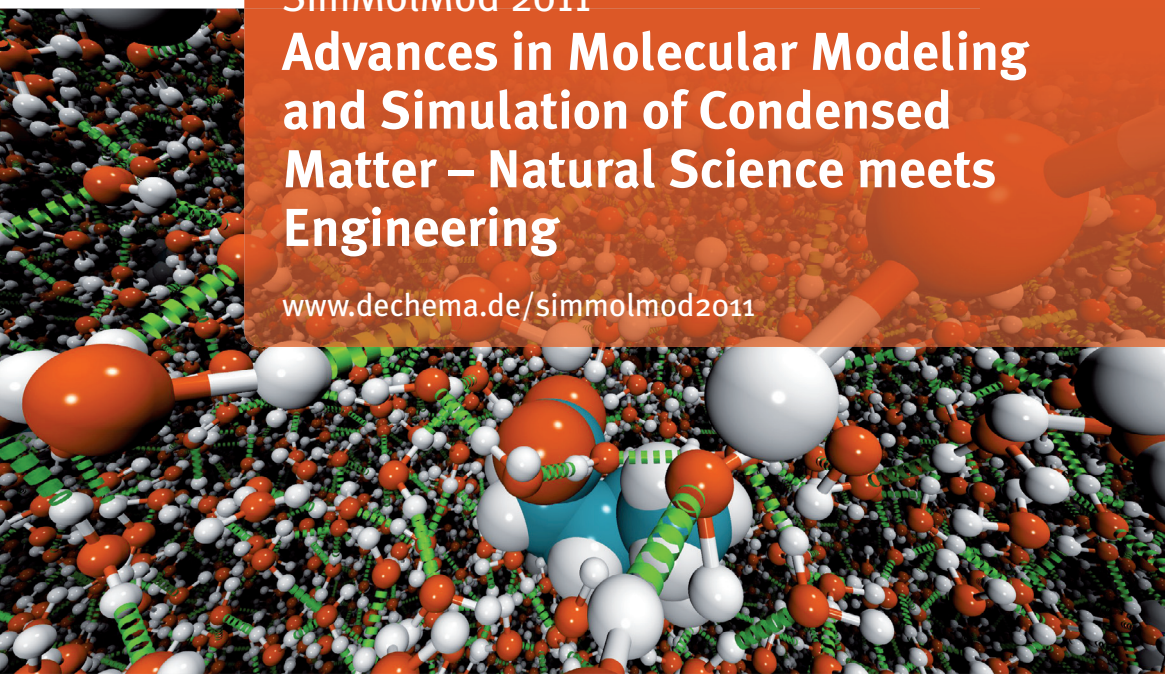
PROGRAMME

September 15 – 16, 2011 · TU Dortmund · Germany

SimMolMod 2011

Advances in Molecular Modeling and Simulation of Condensed Matter – Natural Science meets Engineering

www.dechema.de/simmolmod2011



IN COOPERATION WITH

technische universität
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INVITATION

Molecular modeling and simulation provide insight in the properties of condensed matter also in cases where complex molecules or mixtures are of interest. Moreover, quantitative results are obtained which can be used in engineering for developing new processes and products. Methods on different levels are used, ranging from ab initio quantum chemistry over molecular modeling and simulation with classical force fields to particle-based coarse grained approaches. Bridging these different scales is often the key to yielding the desired results on physico-chemical properties of condensed matter. In order to turn that insight into innovation cooperation between natural science and engineering is needed.

The aim of the present Bunsen Meeting is therefore to strengthen the link between natural science and engineering in the field of molecular modeling and simulation of condensed matter. The focus will be on methods for predicting physico-chemical properties of industrial relevance. Special attention will be given to advances in the methods in the field both from the natural scientists and the engineer's perspective and to creating opportunities for a symbiosis.

SCIENTIFIC COMMITTEE

Hans Hasse	TU Kaiserslautern
Christian Holm	University of Stuttgart
Barbara Kirchner	University of Leipzig
Florian Müller-Plathe	TU Darmstadt
Gabriele Sadowski	TU Dortmund
Jadran Vrabec	University of Paderborn

VENUE

TU Dortmund
Maschinenbaugebäude I,
Hörsaal 1
Leonhard-Euler-Straße
44227 Dortmund

CONFERENCE OFFICE

DECHEMA e.V.
Society for Chemical Engineering and Biotechnology
Attn. Heike Geiling
Theodor-Heuss-Allee 25
60486 Frankfurt am Main/Germany

Office Hours onsite in Dortmund

Thursday, September 15, 2011	12:00 – 18:00
Friday, September 16, 2011	08:30 – 13:00

Thursday, September 15, 2011

11:30	**Lunch** Different options to be paid by the participant himself are available on the campus.
12:00	Registration open
13:00	**Welcome and Introduction** H. Hasse, TU Kaiserslautern/D G. Sadowski, TU Dortmund/D
13:10	**PLENARY LECTURE** **The well-tempered ensemble** M. Parinello, ETH Zürich/CH
13:50	**The process of capillary condensation in a mesopore** H. Morgner, University of Leipzig/D
14:20	**Molecular simulation of transport properties, entrance and confinement effects for real fluids in nanofiltration membranes** M. Horsch, TU Kaiserslautern/D; H. Frentrup, Imperial College, London/UK; S. Becker, TU Kaiserslautern/D; M. Heitzig, University of Stuttgart/D; C. Avendaño Jiménez, E.A. Müller, Imperial College, London/UK; J. Vrabec, University of Paderborn/D; H. Hasse, TU Kaiserslautern/D
14:50	Coffee Break
15:20	**PLENARY LECTURE** **Nano tools for macro problems: multiscale molecular modeling of polymer nanocomposites** M. Fermeglia, Universita di Trieste/I
16:00	**The influence of amino acids on the activity coefficient and structure of water** S. Hempel, G. Sadowski, TU Dortmund/D
16:30	**PLENARY LECTURE** **Development and application of dispersion corrected density functionals** S. Grimme, University of Münster/D
17:10	**Van der Waals-DFT (vdW-DF) investigations of local interfacial interactions between amorphous SiO_2 and supported graphene** F. Keil, A.N. Rudenko, TU Hamburg-Harburg/D
17:40	End of the Lecture Programme
19:00-23:00	**Get Together and Dinner at the Restaurant „Hövels Hausbrauerei“**

Friday, September 16, 2011

9:00	**PLENARY LECTURE** **Molecular simulations of phase equilibrium properties supported by analytic fluid theories** J. Groß, University of Stuttgart/D
9:40	**Combination of molecular dynamic simulations with COSMO-RS: prediction of the partition behavior of different solutes in micelle/water and liposome/water systems** S. Storm, T. Ingram, S. Jakobtorweihen, I. Smirnova, Technology, Hamburg-Harburg/D
10:10	**Quantum chemistry beyond gas phase reactivity: prediction of thermodynamics and kinetics for condensed phase reactions** P. Deglmann, BASF SE, Ludwigshafen/D
10:40	Coffee Break
11:10	**PLENARY LECTURE** **Molecular simulation of phase equilibria and self-assembly: progress and challenges** A. Panagiotopoulos, Princeton University, NJ/USA
11:50	**Reactive molecular dynamics simulations of polymerization** K. Farah, F. Müller-Plathe, M.C. Böhm, TU Darmstadt/D
12:20	**From the inhomogeneous electron gas to classical force fields: multiscale modelling of molecular ionic liquids** F. Dommert, University of Stuttgart/D; K. Wendler, Max-Planck-Institute for Polymer Research, Mainz/D; R. Berger, TU Darmstadt/D; L. Delle Site, Max-Planck-Institute for Polymer Research, Mainz/D; C. Holm, University of Stuttgart/D
12:50	**PLENARY LECTURE** **Mesoscopic simulations of electroosmotic flow and electrophoresis in microfluidics** F. Schmid, University of Mainz/D
13:30	Closing Remarks

Lunch
Different options to be paid by the participant himself are available on the campus.

POSTER PROGRAMME

Posters must be placed on the assigned boards by **Thursday, September 15, 2011, 15:30** at the latest.

Posters will be viewed and discussed during the coffee and lunch breaks.

P 1 **Phase equilibria and interfacial properties of CO_2 mixtures**
G. Niño Amézquita, S. Enders, TU Berlin/D

P 2 **Development of an equation of state based on lattice cluster theory for pure compounds**
K. Langenbach, S. Enders, TU Berlin/D; D. Browarzik, University of Halle-Wittenberg/D

P 3 **IBIsCO: a molecular dynamics simulation package for coarse-grained simulation**
H. Karimi Varzaneh, TU Darmstadt/D; H.-J. Qian, Nagoya University/J; X. Chen, Nanjing University/PRC; P. Carbone, University of Manchester/UK; F. Müller-Plathe, TU Darmstadt/D

P 4 **Combination of COSMO-RS and MD for prediction of partition coefficients in micellar systems**
E. Sponsel, L. Mokrushina, W. Arlt, University of Erlangen-Nuremberg/D

P 5 **„Experiment-based" kinetic Monte-Carlo simulations of CO oxidation over RuO_2(110)**
F. Heß, A. Farkas, H. Over, University of Gießen/D

P 6 **Molecular dynamics investigation of Poly(N-isopropylacrylamide) a thermo-responsive polymer**
M. Alaghemandi, E. Spohr, University of Duisburg-Essen/D

P 7 **Molecular dynamics studies on the reaction system of silicon production using the ReaxFF Reactive Force Field**
J.-P. Mai, G. Raabe, J. Köhler, TU Braunschweig/D

P 8 **Molecular dynamic simulations of the effect of interfacial water on the interaction between nanoparticles**
S. Leroch, M. Wendland, S. Pabisch, H. Peterlik, University of Vienna/A

P 9 **Integration of multi-disciplinary optimisation with molecular simulation**
D. Di Stefano, Esteco srl, Trieste/I; G. Goldbeck, Goldbeck Consulting Ltd, Cambridge/UK

P 10 **Lipid bilayer molecular dynamics simulations for the prediction of partition coefficients**
S. Jakobtorweihen, T. Ingram, S. Storm, F.J. Keil, Hamburg-Harburg/D

P 12 **Computer chemistry of a complex system: interface between biological solution and titanium dioxides**
W. Langel, W. Friedrichs, B. Ohler, Universität Greifswald/D; S. Köppen, Universität Bremen/D

P 13 **Modeling the structure and adsorption properties of titanium passivation layers**
B. Ohler, W. Langel, Universität Greifswald/D

P 14 **Heat storage based on the condensation/evaporation transition of water in pores**
I. Brovchenko, A. Oleinikova, TU Dortmund/D

P 15 **Thermophysical properties of ionic liquid 1-ethyl-3-methyl-imidazolium tetracyanoborate by molecular simulation**
T. Koller, A.P. Fröba, University Erlangen-Nuremberg/D; J. Ramos, BIOPHYM, Madrid/E; I.G. Economou, The Petroleum Institute, Abu Dhabi/UAE

P 16 **Lamellae formation in dissipative particle dynamics simulations: effect of periodicity and finite size of the system**
J. Skvor, Z. Posel, Jan Evangelista Purkinje University, Usti nad Labem/CZ

P 17 **Principal component analysis of dihedral angles as a criterion for the choice of conformations of flexible molecules**
P. Yamin, K. Leonhard, RWTH Aachen University/D; L. Mokrushina, W. Arlt, University of Erlangen-Nuremberg/D

P 18 **MD and QSPR investigations of viscosity in ionic liquids**
S.N. Butler, F. Müller-Plathe, TU Darmstadt/D

P 19 **Formation of polysilsesquioxane and zeolites: a theoretical study**
L. Rutz, O. Deutschmann, H. Bockhorn, Karlsruhe Institute of Technology/D

P 20 **Accurate pair potential for ethylene oxide from quantum chemical ab initio calculations**
J.-P. Crusius, T. Vasiltsova, E. Bich, R. Hellmann, E. Hassel, Universität Rostock/D

P 21 **Scale-relations between critical and near critical phenomena in amorphous and polycrystalline smart materials**
M. Fischelscheiger, TU Berlin/D; E.R. Oberaigner, Montanuniversität, Leoben/A; S. Enders, TU Berlin/D

P 22 **Ab initio equation of state for gaseous and supercritical argon based on the virial expansion**
B. Jäger, R. Hellmann, E. Bich, E. Vogel, University of Rostock/D

P 23 **Simulations of polymer soulutions in an external field:molecular understanding of electrospinning**
I. Nezbeda, J. E. Purkinje University, Prague/CZ

P 24 **Molecular simulation of curved fluid interfaces**
M. Horsch, TU Kaiserslautern/D; J. Vrabec, Universität Paderborn/D; H. Hasse, TU Kaiserslautern/D

P 25 **Reliability of numerical optimization algorithms for the efficient and robust development of molecular models**
M. Hülsmann, K.N. Kirschner, T. Köddermann, D. Reith, Fraunhofer Institute SCAI, Sankt Augustin/D

P 26 **Physico-Chemical properties of a GROW-optimized model for $[C_2MIM][NTf_2]$ via Molecular Dynamics Simulation**
T. Koeddermann, M. Huelsmann, D. Reith, Fraunhofer Institute SCAI, Sankt Augustin/D

P 27 **Molecular simulation of aqueous electrolyte solutions: new force fields for monovalent anions and cations**
S. Deublein, S. Reiser, J. Vrabec, H. Hasse, University of Kaiserslautern/D

P 28 **Molecular simulation of curved fluid interfaces**
M. Horsch, TU Kaiserslautern/D; J. Vrabec, University of Paderborn/D; H. Hasse, TU Kaiserslautern/D

P 29 **Ionic liquids at electrified interfaces and the shape of the capacitance profile from simulations**
N. Georgi, MPI for Mathematics in the Sciences, Leipzig/D

SOCIAL PROGRAMME

Thursday, September 15, 2011	19:00 – 23:00

Get Together and Dinner at the "Hövels Hausbrauerei"

Meeting Point at: Hövels Hausbrauerei, Hoher Wall 5 – 7, 44137 Dortmund

Cost per person: 42,00 € (plus 19% VAT) incl. food and drinks
Registration is required.

REGISTRATION

Please complete the online registration form via **www.dechema.de/simmolmod2011**.

An automatically generated confirmation of receipt will be sent to you by email directly after finishing your online registration. A separate invoice by mail will be sent to you after your registration has been booked in.

In general there is no registration deadline as long as free capacity is available.

Please note: registrations made after **August 23, 2011** are not guaranteed to appear in the list of participants.

REGISTRATION FEES[1)]

Participant	320,00 €
Student (proof of status required)	60,00 €

1) No VAT requested according to § 4.22 UstG

The fee includes the book of abstracts, the list of participants and beverages during the coffee breaks, but no lunch.

REMITTANCE OF FEES

Fees should be remitted on receipt of the invoice in favour of DECHEMA e.V. to one of the DECHEMA accounts as stated on the invoice. When you authorise the payment for our invoice, please be sure to note as the reason for payment our complete invoice number.

CANCELLATIONS AND REFUNDS

30 € for administrative costs will be charged for cancellations received by **August 23, 2011**. Thereafter 80% of the registration fee will be invoiced; however, the book of abstracts will be mailed. Only written cancellations will be accepted. If the event is cancelled by DECHEMA the whole fee will be refunded. Further claims for compensation are excluded.

LUNCH/SNACKS

Lunch and Snacks will be available at the Mensa or in a shop at the TU Dortmund. Participants are expected to pay for their lunch themselves.

INSURANCE

The organizers cannot accept responsibility for loss or damage to the private property of participants and accompanying persons which may occur either during or arising from the conference. Participants should therefore take whatever steps they consider necessary regarding insurance.

HOW TO GET TO / ACCOMMODATION

General information, contact and price details to plan your stay as well as a map and directions how to get to the conference site is available at **www.dechema.de/simmolmod2011**.

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