PROCESSNET

EINE INITIATIVE VON DECHEMA UND VDI-GVC

PROGRAMME

March 11 – 12, 2013

DECHEMA-House · Frankfurt/Main

International Workshop

Molecular Modeling and Simulation: Natural Science meets Engineering

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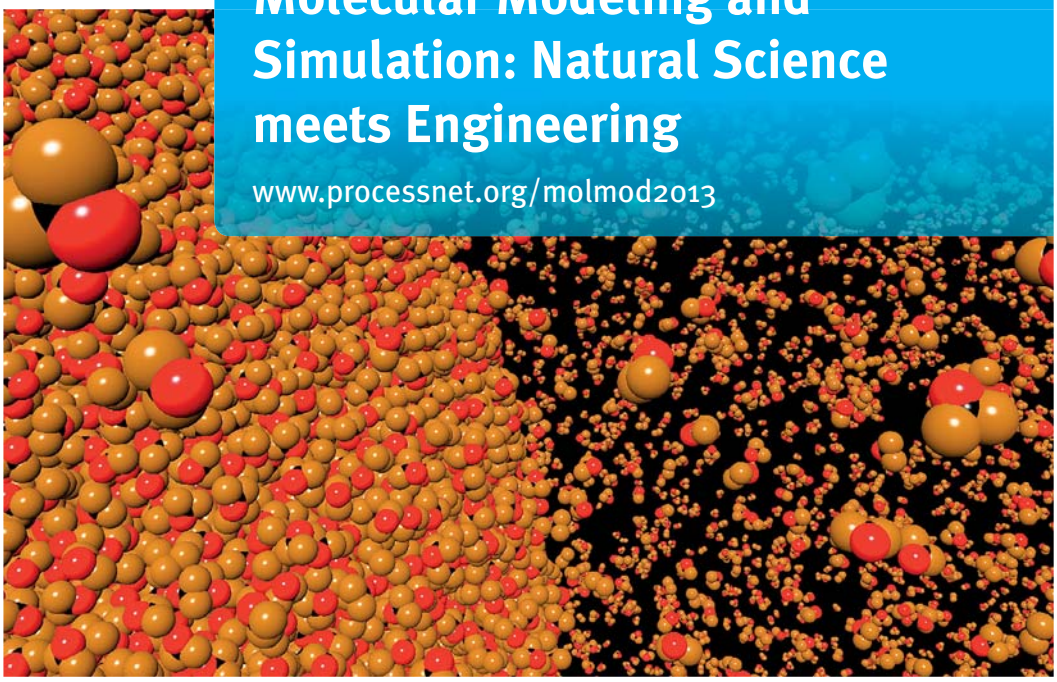

ORGANIZER

DECHEMA VDI

LECTURE PROGRAMME

Monday, March 11, 2013

11:00	Registration, Refreshments
	Room: Franz Patat Hörsaal
12:00	**OPENING REMARKS** (*Vrabec*)
12:10	**INVITED TALK** **G. C. Schatz: Modeling molecules interacting with carbon or gold nanostructures**
12:50	Short break

SESSION A

12:55	**The economic impact of molecular modelling of chemicals and materials** G. Goldbeck
13:15	**Engineering values from computational molecular and materials science** E. Wimmer, M. Yiannourakou, P. Ungerer
13:35	**Efficient combination of environment change and alchemical perturbation in free enthalpy calculations – application to log P determination** N. Hansen, P. H. Hünenberger, W. F. van Gunsteren
13:55	Coffee Break
14:35	**INVITED TALK** **P. Madden: Modelling ionic liquids at interfaces – electrochemistry and supercapacitors**
15:15	Short break
15:20	**Coarse grained molecular dynamics of a ionic liquid-based capacitor: Parameter study on ion size, valency, volume fraction and shape** K. Breitsprecher, P. Košovan, C. Holm
15:40	**Molecular dynamics determination of water-nanorough surfaces interfacial excess free energy** F. Leroy, F. Müller-Plathe
16:00	**Molecular simulation of curved interfaces** M. Horsch, S. Werth, J. Vrabec, H. Hasse
16:20	Coffee Break
16:50	**INVITED TALK** **G. Jackson: Obtaining coarse grained intermolecular potential models for molecular simulation using a third-order perturbation theory: the SAFT-g Mie force field**
17:30	**Poster Party**
20:00	**Social Program – Dinner** (Registration required) Dauth Schneider, Neuer Wall 5 – 7 , 60594 Frankfurt am Main

Monday, March 11, 2013

Room: Paul Duden Raum

SESSION B

12:55	**Temperature dependence of the effective potential between two capped gold nano crystals** G. Bauer, A. Lange, N. Gribova, C. Holm, J. Groß
13:15	**Modeling and calculation of the stacking fault free energy of iron at high temperature** J. Rezaeimianroodi, B. Svendsen
13:35	**The suitability of classical force fields for the molecular modeling of diffusion-limited crystal dissolution processes** M. Greiner
15:20	**Diffusion coefficients of binary and ternary liquids from molecular dynamics simulations** X. Liu, A. Bardow, T.J.H. Vlugt
15:40	**Accurate calculations of partition coefficients (Log POW and Log PMW) with atomistic simulation methods** T. Köddermann, D. Reith, A. Arnold
16:00	**Simulation of lipases in organic solvents: catalytic activity, protein dynamics, and thermodynamic activity** J. Pleiss

Tuesday, March 12, 2013

Room: Franz Patat Hörsaal

9:00	**INVITED TALK** **R. Catlow: Computer modelling as a tool in materials chemistry**
9:40	Short break

SESSION A

9:45	**Molecular simulation of aqueous and non-aqueous electrolyte solutions** S. Reiser, S. Deublein, J. Vrabec, H. Hasse
10:05	**Specific ion effects: molecular simulations of ion pairing, salting-out phenomena and the water solubility of macromolecules** N. van der Vegt
10:25	**Efficient calculation of long-range dispersion interactions using a PPPM Ewald method** R. E. Isele-Holder, F. Key, W. Mitchell, A. E. Ismail
10:45	Coffee Break
11:25	**INVITED TALK** **J. Sauer: *Ab initio* simulation of adsorption isotherms for microporous materials (MOFs, zeolites)**
12:05	Short break
12:10	**Intermolecular force field parameterization from first principles** M. Tafipolsky, B. Engels
12:30	**Transferable force fields for phase equilibria and diffusion coefficients** A. Hemmen, J. Groß
12:50	**Multicriterial optimization of molecular force fields by Pareto approach** K. Stöbener, S. Reiser, M. Horsch, P. Klein, H. Hasse
13:10	Lunch
14:10	**INVITED TALK** **K. Reuter: Towards a first-principles chemical engineering**
14:50	Short break
14:55	**Fundamental equations of state based of hybrid data** G. Rutkai, M. Thol, R. Lustig, R. Span, J. Vrabec
15:15	**Virial equation of state for methane from Mayer-sampling Monte Carlo calculations** R. Hellmann, J.-P. Crusius, T. Vasyltsova, E. Hassel, E. Bich
15:35	**Molecular simulation studies on fluoropropene refrigerants and blends** G. Raabe
15:55	Short break
16:00	**INVITED TALK** **van Gunsteren: Multi-resolution simulation in biochemistry: methodological issues and applications**
16:40	**Concluding Remarks** (*Hasse*)
16:50	End

Tuesday, March 12, 2013

Room: Paul Duden Raum

SESSION B

9:45	**Methods for high performance molecular dynamics** C. W. Glass, C. Niethammer
10:05	**The simulation code Mardyn – Recent developments** W. Eckhardt, A. Heinecke, P. Neumann, H.-J. Bungartz
10:25	**MegaMol – Visualization science for molecular dynamics** S. Grottel, G. Reina
12:10	**N-alkane adsorption and cracking on ZSM-5 and Y zeolite** D. C. Tranca, F. J. Keil
12:30	**Molecular modeling of adsorption phenomena in zeolites: Comparison of model sizes and importance of charge compensations** K. Stückenschneider, J. Merz, G. Schembecker
12:50	**Application of lattice cluster theory for calculating solid-liquid phase equilibria of polymer-solvent systems** M. Fischlschweiger, S. Enders
14:55	**Molecular dynamics simulations of mixed micellar systems for predictions with COSMOmic** S. Storm, S. Jakobtorweihen, I. Smirnova
15:15	**Fluid phase coexistence for the oxidation of cyclohexane in CO_2 expanded liquids: COSMO-SAC vs. molecular simulation** C.-M. Hsieh, T. Merker, S.-T. Lin, H. Hasse, J. Vrabec
15:35	**New features in TRAVIS – The free trajectory analyzer** M. Brehm, M. Thomas, B. Kirchner

POSTER

P 1 **Wettability of solid surfaces: a molecular simulation study**
S. Becker, M. Horsch, H. Hasse

P 2 **Thermophysical properties of gaseous methane-nitrogen mixtures from state-of-the-art *ab initio* pair potentials**
E. Bich, R. Hellmann, E. Vogel

P 3 **ms2: Open source code for molecular simulation of thermodynamic properties of fluids**
S. Deublein, B. Eckl, J. Stoll, S. Lishchuk, G. Guevara-Carrion, C. W. Glass, S. Reiser, T. Merker, T. Windmann, M. Bernreuther, M. Horsch, H. Hasse, J. Vrabec

P 4 **Thermodynamic modeling of phase equilibria in electrolyte systems with COSMO-RS**
T. Gerlach, T. Ingram, T. Mehling, I. Smirnova

P 5 **Kinetic Monte Carlo modeling of the HCl oxidation on RuO_2(110): How far can one get with DFT?**
F. Heß, H. Over

P 6 **Aqueous solutions of inorganic gases by simple molecular models**
J. Jirsak, J. Skvor, I. Nezbeda

P 7 **Quantum chemical high-throughput screening in applied catalysis and functional chemicals development**
A. Kulesza, M. Checinski

P 8 **Molecular dynamics studies on the role of gaseous intermediates in silicon production using the reactive force field ReaxFF-lg**
J.-P. Mai, G. Raabe

P 9 **Hydrogen bonding of ethanol in supercritical mixtures with CO_2 by ^{1}H NMR spectroscopy and molecular simulation**
S. Reiser, N. McCann, M. Horsch, H. Hasse

P 10 **Detection of interfaces and their properties: aqueous slab exposed to external electric field + self-assembled diblock copolymer structures**
J. Skvor, J. Jirsak, Z. Posel, J. Skvara, I. Nezbeda

P 11 **Molecular-level simulation of dew-points of fluid mixtures**
M. Skvorova, I. Nezbeda, W. R. Smith

P 12 **Surface tension of thin films and real fluids**
S. Werth, M. Horsch, H. Hasse

P 13 **Developing a coarse-grained model of an aqueous non-ionic surfactant for the properties of the air-water interface**
C.Herdes, O. Lobanova, E. Santiso, G. Jackson, J. Eastoe, E. A. Müller

P 14 **Simple SPC/E-based models of electrolytes: simulation study on limits of their applicability**
F. Moucka, I. Nezbeda, W. R. Smith

POSTER

P 15 **Methodology for interaction model parameter development: incorporation of concentration dependent data of electrolytes**
F. Moucka, I. Nezbeda, W. R. Smith

P 16 **SAFT-γ Mie approach for the simulation of alkanes with coarse-grained force fields for the intra- and inter-molecular interactions**
S. Rahman, V. Raptis, C. Braga, E. A. Muller, A. Galindo, G. Jackson

P 17 **Molecular dynamics simulations of protein adsorption onto ion-exchange adsorbent: connection to SMA model parameters**
J. Liang, G. Fieg, F. J. Keil, S. Jakobtorweihen

P 18 **Direct simulations of molecular transport and permeation of gases in polymer membrane materials for separation processes**
H. Frentrup, K. E. Hart, C. Colina, E. A. Müller

P 19 **Differential capacitance of coarse-grained ionic liquids**
K. Breitsprecher, P. Kosovan, C. Holm

P 20 **Modelling cellulose dissolution in ionic liquids: insights from statistical analysis of atomistic simulations**
P. Yamin, B. Rabideau, A. E. Ismail, K. Leonhard

P 21 **Molecular dynamics studies of the thermodynamic properties and aggregation of nonionic amphiphilic systems using SAFT coarse grained force field**
O. Lobanova, C. Avendaño, C. Braga, T. Lafitte, C. Herdes, V. Raptis, E. E. Santiso, E. A. Müller, G. Jackson

P 22 **Molecular simulation of seawater desalination using hydrogels**
T. Richter, P. Košovan, C. Holm

P 23 **Simulating peptide – ion interactions: choosing a realistic force field**
J. Kahlen, D. Donadio, C. Peter, K. Kremer

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