DECHEMA

VDI

PROGRAMME

23 – 24 March 2015
DECHEMA-House · Frankfurt/Main · Germany

International Workshop Molecular Modelling and Simulation: Science, Engineering and Industrial Applications

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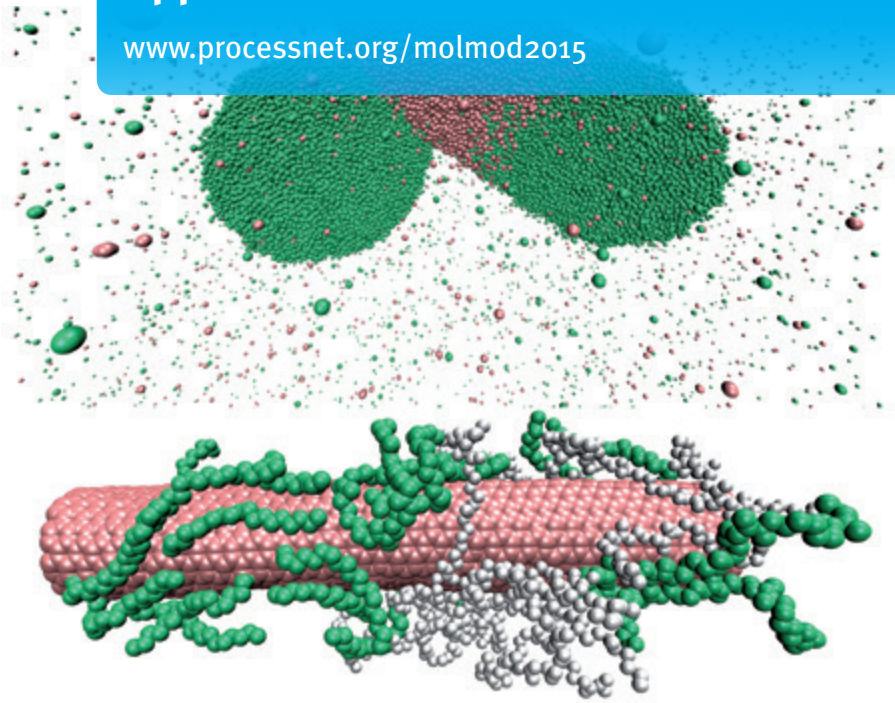

PROCESSNET
EINE INITIATIVE VON DECHEMA UND VDI-GVC

Monday, 23 March 2015

	Max-Buchner-Hörsaal
11:00	Registration, Refreshments
12:00	**Opening Remarks** J. Vrabec, Universität Paderborn/D
12:10	**INVITED TALK** **Multiscale methods for polymeric materials – Mature enough for industry?** F. Müller-Plathe, Technische Universität Darmstadt /D
12:50	Short break
	Max-Buchner-Hörsaal
	SESSION A
12:55	**Integration of mesoscopic and micromechanical modelling for the design of polymer nanocomposites** T. Ozawa, T. Nakayama, M. Watanabe, JSOL Corporation, Tokyo/J; G. Goldbeck, Goldbeck Consulting, Cambridge/UK; V. Regnier, e-Xstream Engineering, Luxembourg/L
13:15	**Crystallisation behaviour of semi-crystalline, branched polyolefines** M. Fischlschweiger, S. Enders, TU Berlin/D
13:35	**Prediction of volumetric and thermodynamic properties of macromolecular solids by atomistic molecular modeling for industrial applications** P. Ungerer, M. Yiannourakou, X. Rozanska, E. Wimmer, A. Mavromaras, V. Eyert, Materials Design S.A.R.L., Montrouge/F; C. Freeman, P. Saxe, MaterialsDesign Inc., Angel Fire/USA
13:55	Coffee Break
14:35	**INVITED TALK** **Combining molecular simulations and advanced analysis tools to enable rapid and reliable thermophysical property prediction** E. Maginn, University of Notre Dame/USA
15:15	Short break

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SESSION B

Molecular simulation studies on HFO working fluids and their blends G. Raabe, TU Braunschweig/D	12:55
Development of new transferable potentials describing phase equilibria for aldehydes, ketones and cyclic alkanes D. Weidler, J. Gross, Universität Stuttgart/D	13:15
Automated global and local optimization methods for atomistic force field development M. Hülsmann, A. Krämer, K. Kirschner, BRS University of Applied Sciences, Sankt Augustin/D; T. Köddermann, Fraunhofer SCAI, Sankt Augustin/D; D. Reith, BRS University of Applied Sciences, Sankt Augustin/D	13:35
Coffee Break	13:55

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SESSION A

15:20	**Molecular simulation based fundamental equations of state** G. Rutkai, Universität Paderborn/D
15:40	**Large-scale molecular dynamics simulation of heterogeneous systems with ls1 mardyn** M. Horsch, R. Srivastava, S. Werth, TU Kaiserslautern/D; C. Niethammer, C.W. Glass, Höchstleistungsrechenzentrum Stuttgart/D; W. Eckhardt, A. Heinecke, N. Tchipev, H.-J. Bungartz, TU München/D; S. Eckelsbach, J. Vrabec, Universität Paderborn/D; H. Hasse, TU Kaiserslautern/D
16:00	**Molecular simulation of organic electrolyte solutions** M. Kohns, R. Steffen, M. Horsch, H. Hasse, TU Kaiserslautern/D
16.20	**The European Materials Modelling Council** G. Goldbeck, Goldbeck Consulting Ltd, Cambridge/UK; N. Adamovic, TU Wien/A; P. Asinari, Politecnico di Torino/I; A. Hashibon, Fraunhofer Institute for Mechanics of Materials IWM, Freiburg/D; K. Hermansson, University of Uppsala/S; P. Klein, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern/D; R. Koopmans, Dow Chemical Company, Horgen/CH
16:40	Coffee Break
17:10	**INVITED TALK** **Molecular simulation of absorption of precombustion gasses in ionic liquids and other solvents** T.J.H. Vlugt, Delft University of Technology/NL
17:50	**Poster Party**
20:00	**Social Programme – Dinner** Dauth-Schneider, Neuer Wall 5-7, 60594 Frankfurt am Main

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SESSION B	
Complex surface-solute model: Biomolecules on contaminated titanium surfaces W. Friedrichs, W. Langel, Universität Greifswald/D	15:20
Molecular-scale behavior of superspreading agents R.E. Isele-Holder, A.E. Ismail, RWTH Aachen/D	15:40
Wetting, adsorption, and contact line pinning by molecular dynamics simulation S. Becker, M. Horsch, H. Hasse, TU Kaiserslautern/D	16:00
Some properties of 1,3 dicarbonyl compounds C. Taeschler, Chemicals R&D/CH	16.20
Coffee Break	16:40
	17:10
Poster Party	17:50
Social Programme – Dinner Dauth-Schneider, Neuer Wall 5-7, 60594 Frankfurt am Main	20:00

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9:00	**INVITED TALK** **Water. What can we learn from computer simulations?** C. Vega de las Heras, University Complutense of Madrid/E
9:40	Short break

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	SESSION A
9:45	**Quantum mechanics in a glass of liquid water** T. Kühne, Universität Paderborn/D
10:05	**Determination of reaction pathways, rates and transition states using reactive molecular dynamics simulations** M. Döntgen, M.-D. Przybylski-Freund, L.C. Kröger, W.A. Kopp, A.E. Ismail, K. Leonhard, RWTH Aachen/D
10:25	**Shifting balance - Experiments, computers, and simulations** J. Lenhard, Universität Bielefeld/D
10:45	Coffee Break
11:25	**INVITED TALK** **A review of the application of quantum calculations in the chemical industry** A. Schäfer, BASF Ludwigshafen/D
12:05	Short break
12:10	**Methanol oxidation to formaldehyde on VEBA zeolite. A combined DFT/transition path sampling – experimental study** D. Tranca, F. Keil, TU Hamburg-Harburg/D; F. Tielens, Paris Sorbonne/F
12:30	**Ab-initio catalyst modelling on the atomic scale: Kinetic Monte Carlo simulations in fundamental heterogeneous catalysis research** F. Hess, H. Over, Universität Gießen/D
12:50	**Molecular simulation of enzymes under realistic reaction conditions** T. Kulschewski, S. Benson, J. Pleiss, Universität Stuttgart/D
13:10	Lunch

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SESSION B

Combining molecular simulations and crystal chemistry: Prediction of promising zeolite frameworks for adsorption applications M. Fischer, University of Bremen/D; R. G. Bell, University College London/UK	9:45
Calculation and microscopic understanding of solid-liquid work of adhesion F. Leroy, TU Darmstadt/D	10:05
Investigating the influence of water on carbon dioxide adsorption and diffusion in Mg-MOF-74 using molecular simulations S. Bendt, Y. Dong, A.N. Rudenko, F.J. Keil, TU Hamburg-Harburg/D	10:25
Coffee Break	10:45
	11:25
	12:05
Application of computer simulations: Molecular insight into electrospinnig I. Nezbeda, F. Moucka, J. Jirsak, J. E. Purkinje University Usti nad Labem/CZ	12:10
Coupled PIC-DSMC simulation of laser driven ablative gas expansions S.M. Copplestone, C.-D. Munz, Universität Stuttgart/D	12:30
Prediction of interfacial properties of industrially relevant fluid mixtures by molecular simulation and density gradient theory + PC-SAFT S. Werth, K. Langenbach, M. Horsch, H. Hasse, TU Kaiserslautern/D	12:50
Lunch	13:10

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14:10	**INVITED TALK** **A priori prediction of phase behaviors of ionic liquids** S.-T. Lin, National Taiwan University/RC
14:50	Short break

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	SESSION A
14:55	**Molecular dynamics simulations of triton X-114 and surfactant mixtures self-assembly and prediction of partition equilibria** D. Yordanova, I. Smirnova, S. Jakobtorweihen, Hamburg University of Technology/D
15:15	**Biomembrane/water partition behavior predictions with molecular dynamics simulations** S. Jakobtorweihen, I. Smirnova, Hamburg University of Technology/D
15:35	**Accurate calculations of partition coefficients (log P_OW and log P_MW) with atomistic simulation methods** T. Köddermann, A. Maaß, Fraunhofer SCAI, Sankt Augustin/D; M. Hülsmann, D. Reith, BRS University of Applied Sciences, Sankt Augustin/D
15:55	Short break
16:00	**INVITED TALK** **Equilibration of high molecular-weight polymer melts: A hierarchical universal strategy** K. Kremer, Max-Planck Institut für Polymerforschung, Mainz/D
16:40	**Concluding Remarks**
16:50	End

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SESSION B

High performance molecular simulation – Complex codes meet evolving hardware C.W. Glass, High Performance Computing Center Stuttgart/D	14:55
Feature-preserving and consistent molecular dynamics visualization G. Reina, Universität Stuttgart/D	15:15
Extending the vectorization of ls1-mardyn N. Tchipev, W. Eckhardt, P. Neumann, H.-J. Bungartz, TU München, Garching b. München/D	15:35
Short break	15:55

POSTER

P.1 **Determining the superstructure of nano crystals**
G. Bauer, A. Lange, N. Gribova, C. Holm, J. Groß, Universität Stuttgart/D

P.2 **Atomistic simulations of supramolecular complexes in aqueous solution**
J. Baz, N. Hansen, Universität Stuttgart/D

P.3 **Retrieving (visco-)elastic properties of homopolymers using DPD**
S. Echeverri Restrepo, SKF, Nieuwegein/NL; F.O. Valega Mackenzie, TNO, Eindhoven/NL

P.4 **Force field validation for the simulation of inclusion complexes of linear alcohols with alpha-cyclodextrin**
J. Gebhardt, D. Markthaler, N. Hansen, Universität Stuttgart/D

P.5 **Calculation of relative folding free enthalpies of amide-to-ester mutations of protein Pin1**
D. Markthaler, N. Hansen, Universität Stuttgart/D

P.6 **Experimental and simulation results for various thermodynamic properties of CO_2/CH_4 mixtures**
M. Schenk, BRS University of Applied Sciences, Sankt Augustin/D; S. Knauer, Eurotechnica, Bargteheide/D; M. Hülsmann, D. Reith, BRS University of Applied Sciences, Sankt Augustin/D; T. Köddermann, Fraunhofer SCAI, Sankt Augustin/D

P.7 **Development of a dynamic cutoff method and interface detection algorithm for long-range dispersion interactions**
P. Springer, P. Bientinesi, B. Berkels, A.E. Ismail, RWTH Aachen/D

P.8 **Characterization of aklylsilane self assembling monolayers by molecular simulation**
J. Castillo Sanchez, Universität Kaiserslautern/D; M. Klos, Universität des Saarlandes, Saarbrücken/D; M. Horsch, Universität Kaiserslautern/D; K. Jacobs, Universität des Saarlandes, Saarbrücken/D; H. Hasse, Universität Kaiserslautern/D

P.9 **Surface tension of real quadrupolar fluids by molecular simulation: prediction and optimization**
S. Werth, TU Kaiserslautern/D; K. Stöbener, Fraunhofer Institute for Industrial Mathematics, Kaiserslautern/D; M. Horsch, H. Hasse, TU Kaiserslautern/D

P.10 **Molecular modelling of nitrous oxide and its application in the CO_2-N_2O analogy**
M. Kohns, E. von Harbou, M. Horsch, H. Hasse, TU Kaiserslautern/D

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