DECHEMA

VDI

PROGRAMME

1 – 2 March 2021 · Online Event

International Workshop on Molecular Modeling and Simulation

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PROCESSNET

EINE INITIATIVE VON DECHEMA UND VDI-GVC

PROGRAMME

Monday, 1 March 2021

Chair: J. Vrabec, TU Berlin/D

10:00 **PLENARY LECTURE**
Dynamics and transport at and through interfaces by molecular dynamics simulation
J. Simon[1]; [1] CNRS-Université de Bourgogne, Dijon/F

OPENING SESSION

Chair: J. Vrabec, TU Berlin/D

10:40 **Transport properties of fluid mixtures at near critical conditions by molecular simulation**
G. Guevara Carrion[1]; J. Vrabec[2]; [1] TU Berlin / Institut für Prozess- und Verfahrenstechnik (FG Dynamik und Betrieb technischer Anlagen), Berlin/D; [2] TU Berlin/D

11:00 **Computational Investigation of the Soret Coefficient in the Context of Host/Ligand Binding**
D. Markthaler[1]; S. Mohankumar[2]; S. Wiegand[2]; N. Hansen[1]; [1] University of Stuttgart/D; [2] Forschungszentrum Jülich GmbH, Jülich/D

11:20 Break

IONIC SYSTEMS

Chair: S. Stephan, TU Kaiserslautern/D

11:40 **NaCl precipitate nucleation from aqueous solution: a simple system holding some surprises**
N. Zimmermann[1]; [1] Hamburg University of Technology, Hamburg/D

12:00 **ChemTraYzing Ionic Liquids**
W. Kopp[1]; F. Schmalz[1]; D. Mehlis[1]; M. Papusha[1]; K. Leonhard[1]; [1] RWTH Aachen University, Aachen/D

12:20 **Molecular Thermodynamics Approach to the Relative Permittivity**
M. Kohns[1]; J. Marx[1]; K. Langenbach[2]; [1] Technische Universität Kaiserslautern/D; [2] Universität Innsbruck/A

12:40 Lunch break

PROGRAMME

Monday, 1 March 2021

MACROMOLECULES

Chair: M. Kohns, TU Kaiserslautern/D

13:40 **Designing compatibilizers for polymer blends: A dissipative dynamics study**
T. Zhou[1]; J. Gámez[2]; F. Müller-Plathe[1]; [1] Technische Universität Darmstadt/D; [2] Covestro Deutschland AG, Leverkusen/D

14:00 **Multiscale modeling of the structural formation in biological macromolecular systems using data-driven coupling**
P. Depta[1]; U. Jandt[2]; C. Jacobi[1]; M. Dosta[1]; A. Zeng[1]; S. Heinrich[1]; [1] Hamburg University of Technology, Hamburg/D; [2] Deutsches Elektronen-Synchrotron DESY, Hamburg/D

POLAR FLUIDS

Chair: K. Leonhard, RWTH Aachen University/D

14:20 **Molecular Orientation Structure and Thermodynamics in Mixtures of Fluids with Different Polarity**
J. Marx[1]; K. Langenbach[1]; [1] University of Innsbruck, Innsbruck/A

14:40 **Multi-criteria Optimisation of Molecular Models of Water**
A. Kulkarni[1]; M. Bortz[2]; K. Küfer[2]; M. Kohns[1]; H. Hasse[1]; [1] Technische Universität Kaiserslautern, Lehrstuhl für Thermodynamik, Kaiserslautern/D; [2] Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern/D

15:00 Break

Chair: J. Vrabec, TU Berlin/D; M. Horsch, High Performance Computing Center Stuttgart/D

15:20 **Poster short presentations**

16:20 **Digital Poster Foyer** (16:20 – 17:30)

PROGRAMME

Tuesday, 2 March 2021

INTERFACE PROCESSES I

Chair: M. Horsch, High Performance Computing Center Stuttgart/D

09:40 **Mass Flux Through Vapor-Liquid Interfaces: A Molecular Simulation Study**
D. Schaefer[1]; S. Stephan[1]; K. Langenbach[1]; H. Hasse[1]; [1] TU Kaiserslautern/D

10:00 **Large scale molecular dynamics simulations and phase-field modeling of droplet coalescence**
J. Vrabec[1]; M. Heinen[1]; [1] TU Berlin/D

10:20 **Atomistic Simulation and Classical Density Functional Theory for Modeling Adsorption in Covalent Organic Frameworks**
C. Keßler[1]; J. Eller[1]; N. Hansen[1]; J. Groß[1]; [1] Universität Stuttgart, Institut für Technische Thermodynamik und Thermische Verfahrenstechnik, Stuttgart/D

10:40 Break

INTERFACE PROCESSES II

Chair: K. Langenbach, Universität Innsbruck/D

11:00 **Properties of Vapor-Liquid Interfaces: Molecular Simulations, Density Gradient Theory, and Experiments**
O. Großmann[1]; S. Stephan[1]; K. Langenbach[1]; H. Hasse[1]; [1] TU Kaiserslautern/D

11:20 **Investigating evaporation processes with large molecular dynamics simulations**
S. Homes[1]; J. Vrabec[1]; [1] TU Berlin/D

11:40 **Molecular Dynamics Simulations of Lubricated Contact Processes on the Nanoscale**
S. Schmitt[1]; S. Stephan[1]; H. Hasse[1]; [1]TU Kaiserslautern/D

12:00 End of the event

POSTER

P 1.01 **A Molecular Model for Poly(oxymethylene) Dimethyl Ethers (OME)**
A. Kulkarni[1]; E. Garcia[1]; A. Damone[1]; M. Schappals[1]; S. Stephan[1]; M. Kohns[1]; H. Hasse[1]; [1] Technische Universität Kaiserslautern, Lehrstuhl für Thermodynamik, Kaiserslautern/D

P 1.02 **Transferable anisotropic Mie-potential force field for amines**
M. Fleck[1]; [1] , Stuttgart/D

P 1.03 **A Database for Molecular Models for the Simulation of Thermodynamic Properties of Fluids**
S. Stephan[1]; M. Horsch[2]; J. Vrabec[3]; H. Hasse[1]; [1] TU Kaiserslautern/D; [2] Daresbury Laboratory, Daresbury/UK; [3] TU Berlin/D

P 1.04 **Automatic PES mapping from Reaxff simulations with ChemTraYzer**
C. Huang[1]; F. Schmalz[1]; W. Kopp[1]; L. Krep[1]; L. Kröger[1]; M. Döntgen[1]; K. Leonhard[1]; [1] RWTH Aachen university, Aachen/D

P 1.05 **Robust Transition State searches based on reactive Molecular Dynamics trajectories**
L. Krep[1]; F. Schmalz[1]; K. Leonhard[1]; [1] RWTH Aachen University, Aachen/D

P 1.06 **An atomistic view on liquid phase adsorption**
H. Kraus[1]; N. Hansen[1]; [1] Universität Stuttgart, Institut für Technische Thermodynamik und Thermische Verfahrenstechnik, Stuttgart/D

P 1.07 **Novel insights into the behavior of alcohol dehydrogenases in deep eutectic solvents: a molecular dynamics study**
J. Bittner[1]; L. Huang[2]; P. Domínguez de María[3]; S. Kara[2]; S. Jakobtorweihen[1]; [1] Hamburg University of Technology, Hamburg/D; [2] Aarhus University, Aarhus/DK; [3] Sustainable Momentum S.L., Las Palmas de Gran Carnaria/E

P 1.08 **Predictive models for the phase behaviour and solution properties of weak electrolytes: nitric, sulfuric and carbonic acids**
M. Kohns[1]; S. Kournopoulos[2]; S. Di Lecce[2]; G. Lazarou[2]; E. Forte[2]; F. Perdomo Hurtado[2]; G. Jackson[2]; C. Adjiman[2]; A. Galindo[2]; [1] Technische Universität Kaiserslautern/D; [2] Imperial College London/UK

P 1.09 **How does the size of the simulation volume impact adsorption simulations near fluid-mixture dew points?**
M. Sekulla[1]; M. Richter[1]; [1] TU Chemnitz/D

P 1.10 **Wetting and Adsorption of Binary Mixtures on a Planar Wall**
J. Staubach[1]; M. Heier[1]; S. Stephan[1]; K. Langenbach[1]; H. Hasse[1]; [1] TU Kaiserslautern/D

P 1.11 **Interfacial properties of polar mixtures: a study by molecular dynamics simulation and density gradient theory**
J. Staubach[1]; S. Stephan[1]; H. Hasse[1]; [1] TU Kaiserslautern/D

P 1.12 **Fundamental Investigation of Electrochemical Synthesis of 2-Methylfuran from Furfural by Molecular Dynamics Simulation**
S. Rabet[1]; A. Mecklenfeld[1]; G. Raabe[1]; [1] Technische Universität Braunschweig/D

POSTER

P 1.13 **The Lennard-Jones potential revisited: reliability and reproducibility or molecular simulation data**
S. Stephan[1]; J. Staubach[1]; U. Deiters[2]; J. Vrabec[3]; H. Hasse[1]; [1] TU Kaiserslautern/D; [2] University of Cologne, Köln/D; [3] TU Berlin/D

P 1.14 **A comparison of classical force fields for the prediction of transport properties of lubricants**
S. Schmitt[1]; S. Stephan[1]; H. Hasse[1]; [1] TU Kaiserslautern/D

P 1.15 **Modeling phosphorylation by human Thymidine Kinase 1. A crucial step in the rational design of thymidine-analogue radiosensitizers. Part I: MD.**
S. Romanowska[1]; Z. Cournia[2]; J. Rak; [1] University of Gdansk/PL; [2] Biomedical Research Foundation, Athens/GR

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