DECHEMA
Gesellschaft für Chemische Technik
und Biotechnologie e.V.

PROGRAMME

24 - 25 February 2025
DECHEMA-Haus · Frankfurt am Main

International Workshop on Molecular Modeling and Simulation

https://dechema.de/MolMod2025

SCIENTIFIC COMMITTEE

DECHEMA Subject Division Molecular Modeling and Simulation for Process and Product Design

Chairman: Prof. J. Vrabec, TU Berlin/D

Monday, 24 February 2025

	Room: Franz-Patat-Hörsaal
11:50	**Welcome by the Chairmen** *Chair: Prof. Jadran Vrabec, TU Berlin/D*
	SESSION "FIRST PRINCIPLES" *Chair: Prof. Jadran Vrabec, TU Berlin*
11:55	**Cross second virial coefficients for mixtures of hydrogen with six common gases from first-principles calculations** Robert Hellmann[1] [1] Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg, Hamburg/DE
12:20	**Thermodynamic properties of quantum fluids: Path integral Monte Carlo simulations of helium and neon using ab initio potentials** Philipp Marienhagen[1]; Karsten Meier[1] [1] Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg, Hamburg/DE
12:45	**Fast and accurate adsorption calculation using the GPU-accelerated classical density functional theory for high-throughput screening and process modelling of paraffin/olefin separation** Tiong Wei Teh[1]; Rolf Stierle[1]; Niels Hansen[1]; Joachim Gross[1] [1] University of Stuttgart, Germany, Stuttgart/DE
13:10	Lunch Break
	SESSION "FUNDAMENTALS" *Chair: Dr. Robert Hellmann,* *Helmut-Schmidt-Universität / Universität der Bundeswehr, Hamburg*
14:10	**Sampling statistical ensembles and three-body interactions with ms2** Isabel Nitzke[1]; Jadran Vrabec[2] [1] TU Berlin , Berlin/DE; [2] Technische Universität Berlin, Berlin/DE
14:35	**Optimizing Interface Force Fields for Water on Platinum (111)** Aditya Kale[1]; Gabriele Raabe[1] [1] Institut für Thermodynamik, TU Braunschweig, Braunschweig/DE
15:00	**Substitute Molecular Dynamics Simulations with a Surrogate Model in a Multi-Scale Force-Field Parameter Optimization** Robin Strickstrock[1]; Alexander Hagg[1]; Yoorim Gye[1]; Dirk Reith[1]; Karl N. Kirschner[1] [1] Hochschule Bonn-Rhein-Sieg, Sankt Augustin/DE
15:25	Coffee Break

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Monday, 24 February 2025

	SESSION "COSMO METHODS" *Chair: Prof. Simon Stephan, RPTU Kaiserslautern*
15:55	**COSMOPharm: Assessment of the Predictive Power of COSMO-SAC for Pharmaceutical Amorphous Solid Dispersions** Ivan Antolovic[1] [1] Technische Universität Berlin, Berlin/DE
16:20	**A comprehensive approach to incorporating intermolecular dispersion into the openCOSMO-RS model. Part 2: Atomic polarizabilities** D. Grigorash[1]; Simon Müller[2]; P. Paricaud[3]; W. Yan[1]; E. H. Stenby[1]; I. Smirnova[2] [1] Danish Technical University, Lyngby/DK; [2] Hamburg University of Technology, Hamburg/DE; [3] ENSTA Paris, Institut Polytechnique de Paris, Palaiseau/FR
16:45 - 17:05	**Short Presentations of Posters** *Chair: Prof. Jadran Vrabec, TU Berlin*
17:05- 18:15	**Poster Party with Beer & Pretzels**
17:45- 18:30	**Advisory Board Meeting** (Invitation only)
19:15- 22:30	**Networking Dinner at Dauth Schneider** (Frankfurt-Sachsenhausen)

Tuesday, 25 February 2025

	Room: Franz-Patat-Hörsaal
	SESSION "BATTERIES & PROTEINS" *Chair: Dr. Gabriela Guevara Carrión, TU Berlin*
09:00	**Advanced carbon aerogels for battery applications: A molecular study** Hemangi Patel[1]; Jessica Kröner[1]; Marina Schwan[1]; Barbara Milow[1]; Ameya Rege[2] [1] DLR (Deutsches Zentrum für Luft- und Raumfahrt), Köln/DE; [2] University of Twente, Enschede/NL
09:25	**Molecular characterization of organic active materials for redox-flow-batteries** Miriam Sprick[1]; Eduardo Schneider[1]; Waldemar Dann[1]; Gabriele Raabe[1] [1] Technische Universität Braunschweig, Braunschweig/DE
09:50	**Calculation of a two-dimensional free energy surface for protein adsorption** Marius Fiedler[1]; Thomas Waluga[1]; Irina Smirnova[1]; Sven Jakobtorweihen[1] [1] Technische Universität Hamburg, Hamburg/DE
10:15	Coffee Break

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Tuesday, 25 February 2025

	SESSION "EQUATIONS & TRANSPORT" *Chair: Prof. Simon Stephan, RPTU Kaiserslautern*
10:45	**Equation of State Modeling and Molecular Simulation of polar interactions** Xueqi Zhang[1] [1] RPTU Kaiserslautern, Kaiserslautern/DE
11:10	**Modeling Transport Properties of Fluids using Molecular-based Equations of State – An Entropy Scaling Framework** Dennis Alt[1]; Sebastian Schmitt[1]; Hans Hasse[1]; Simon Stephan[1] [1] RPTU Kaiserslautern, Kaiserslautern/DE
11:35	**Thermodynamic properties of the Lennard-Jones fluids in N dimensions** Simon Homes[1] [1] TU Berlin , Berlin/DE
12:00	**Transport properties of the Lennard-Jones fluid: Database and data assessment** Florian Fleckenstein[1]; Sebastian Schmitt[1]; Jadran Vrabec[2]; Hans Hasse[1]; Simon Stephan[1] [1] RPTU Kaiserslautern-Landau, Kaiserslautern/DE; [2] TU Berlin, Berlin/DE
12:25	**Transport diffusion of aqueous alkali halide solutions by molecular simulation** Gabriela Guevara-Carrion[1]; Jadran Vrabec[1] [1] TU Berlin, Berlin/DE
12:50	Lunch Break
	SESSION "POROUS MATERIALS" *Chair: Prof. Jadran Vrabec, TU Berlin*
13:50	**From spheres to real molecules: Adsorption of gases in nanoporous materials with classical density functional theory** Philipp Rehner[1] [1] Energy and Process Systems Engineering, ETH Zürich | Switzerland /CH
14:15	**Molecular dynamics simulation study of slip mechanism at solid-fluid interfaces** Raihan Alfaridzi[1]; Yudi Rosandi[2]; Simon Stephan[1]; Herbert M. Urbassek[1] [1] RPTU - Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Kaiserslautern/DE; [2] Universitas Padjadjaran, Jatinangor/ID
14:40	**Confinement Effects in Mesopores Studied by Molecular Dynamics Simulations** Marc Högler[1]; Hamzeh Kraus[1]; Niels Hansen[1] [1] University of Stuttgart, Stuttgart/DE

POSTER

P 01	**Coupling molecular thermodynamics models with CFD simulation engines** Xueqi Zhang[1] [1] RPTU Kaiserslautern, Kaiserslautern/DE
P 02	**MolMod: A Force Field Database for Molecular Simulation of Fluids** Florian Fleckenstein[1]; Sebastian Schmitt[1]; Hans Hasse[1]; Simon Stephan[1] [1] RPTU Kaiserslautern-Landau, Kaiserslautern/DE
P 03	**Development of methodologies for a rational design of enzymatic catalytic reaction cascades** Eduardo Schneider[1]; Miriam Sprick[1]; Carla Matke[1]; Gabriele Raabe[1] [1] Institut für Thermodynamik, TU Braunschweig/DE
P 04	**Molecular study on the formation of porous silica networks in an all-atom-approach** Katharina Lauchner[1,2]; Hemangi Patel [1,2]; Barbara Milow [1,2]; Ameya Rege [1,3] [1] German Aerospace Center (DLR), Institute of Materials Research, Cologne/DE [2] University of Cologne, Institute of Inorganic and Materials Chemistry, Cologne/DE [3] University of Twente, Department of Mechanics of Solids, Surfaces & Systems, Enschede/NL

ORGANISER / CONTACT

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