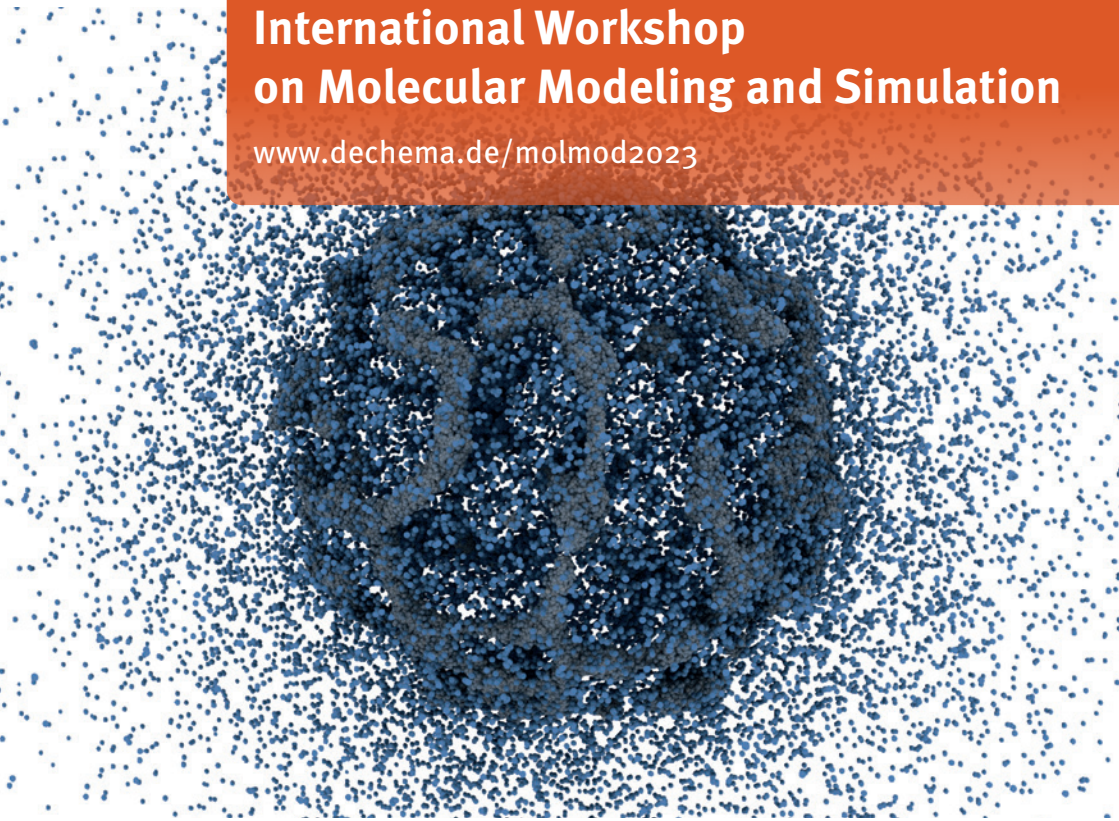
DECHEMA

PROGRAMME

2 – 3 March 2023 · DECHEMA-Haus · Frankfurt am Main

International Workshop on Molecular Modeling and Simulation

www.dechema.de/molmod2023



GENERAL INFORMATION

VENUE

DECHEMA-Haus
Theodor-Heuss-Allee 25
60486 Frankfurt am Main
Germany

COMMITTEE

Prof. J. Vrabec TU Berlin/D
Dr. N. Möller DECHEMA e.V., Frankfurt am Main/D

ORGANIZER / CONTACT

DECHEMA e.V.
Theodor-Heuss-Allee 25
60486 Frankfurt am Main
Germany

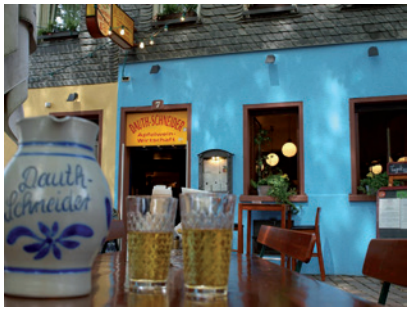
Sabine Urbanczyk
Tel.: 0049 (0)69 -7564-295
E-Mail: sabine.urbanczyk@dechema.de

SOCIAL PROGRAMME

Thursday, 2 March 2023 **19:30 – 22:00 h**

Get together "Geselliger Abend" in the Restaurant Dauth-Schneider
on a self-pay basis

Apfelweinwirtschaft Dauth-Schneider
Neuer Wall 5-7, Klappergasse 39
60594 Frankfurt am Main
www.dauth-schneider.de



As of February 2023
Programme is subject to alternations. Submission title and authors information as provided by the submitter. No proof by DECHEMA.

PROGRAMME

Thursday, 2 March 2023

Room: Franz-Patat-Hörsaal

11:55	**Welcome**
12:00	**PLENARY LECTURE** **How does the gecko run on almost any surface? Lessons from multi-scale molecular simulation** F. Müller-Plathe[1]; [1] Technische Universität Darmstadt/D
	FUNDAMENTALS
12:40	**On the history, ontology, and computation of the Lennard-Jones fluid** J. Lenhard[1]; S. Stephan[1]; H. Hasse[1]; [1] TU Kaiserslautern/D
13:00	**Thermophysical properties of oxygen gas from first principles** R. Hellmann[1]; [1] Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg/D
13:20	**Assessing thermodynamic properties in all ensembles** I. Nitzke[1]; J. Vrabec[1]; [1] TU Berlin/D
13:40	Coffee break
	NON-EQUILIBRIUM MD/PHASE TRANSITIONS
14:20	**ls 1 mardyn and AutoPas – Advancements of the massively parallel, auto-tuned simulation framework for large-scale molecular systems** F. Hoppe[1]; A. Das Sharma[1]; P. Neumann[1]; F. Gratl[2]; [1] Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg/D; [2] Technical University of Munich/D
14:40	**Interface resistivities of vapor-liquid interfaces** S. Homes[1], J. Vrabec[1]; [1] TU Berlin/D
15:00	**Characteristics of Droplet Explosions Studied with Non-Equilibrium Molecular Dynamics Simulations** D. Schaefer[1]; B. Kunstmann[1]; S. Schmitt[1]; M. Kohns[1]; H. Hasse[1]; [1] TU Kaiserslautern/D
15:20	**Beyond Periodic Boundary Conditions: Force Field Simulations of the "Breathing" Phase Transformation of MOF Nanocrystallites** L. Schaper[1]; J. Keupp[1]; R. Schmid[1]; [1] Ruhr-Universität Bochum/D
15:40	Coffee break
	POLYMERS
16:10	**Simulating the Influence of Polymer-Aroma Interactions on Perceived Aroma in Red Wine** T. Koch[1]; A. Gabler[1]; J. Kreißl[1]; O. Frank[1]; H. Briesen[1]; [1] Technical University of Munich, Freising/D
16:30	**Microstructure in Highly Stretched Polyethylene Systems** D. Grommes[1]; M. Schenk[1]; O. Bruch[2]; D. Reith[1]; [1] Bonn-Rhein-Sieg University of Applied Sciences, Sankt Augustin/D; [2] Dr. Reinold Hagen Stiftung, Bonn/D
16:50	**Poster Presentations**
17:50	**Poster Party** (17:50 – 18:50)
19:30 – 22:00	**Get together "Geselliger Abend" in the Restaurant Dauth-Schneider** on a self-pay basis (www.dauth-schneider.de)

PROGRAMME

Friday, 3 March 2023

Room: Franz-Patat-Hörsaal

TRANSPORT

09:00 **Diffusion in supercritical CO_2 mixtures**
D. Saric[1]; G. Guevara-Carrión[1]; J. Vrabec[1]; V. Shevtsova[2]; [1] TU Berlin/D; [2] Mondragon Unibertsitatea, Arrasate-Mondragon/E

09:20 **Transport properties of pure components and mixtures: Predictions from molecular simulation and entropy scaling**
D. Fertig[1]; S. Schmitt[1]; H. Hasse[1]; S. Stephan[1]; [1] Technische Universität Kaiserlautern/D

09:40 **Transport at the upper critial point of the liquid-liquid equilibrium**
I. Antolovic[1]; J. Staubach[2]; S. Stephan[2]; J. Vrabec[1]; [1] Technische Universität Berlin/D; [2] Technische Universität Kaiserlautern/D

10:00 Coffee break

FORCE FIELDS

10:40 **Machine learning assisted Monte Carlo simulation of non-spherical particles**
S. Bag[1]; [1] Technical University of Darmstadt/D

11:00 **Transferable Force Fields and Transport Properties**
M. Fleck[1]; N. Hansen[1]; J. Gross[1]; [1] Universität Stuttgart/D

11:20 **Hierarchical Multi-criteria Optimisation of Molecular Models of Water Using Five Objectives**
M. Kohns[1]; A. Kulkarni[1]; M. Bortz[2]; K. Küfer[2]; H. Hasse[1]; [1] TU Kaiserslautern/D; [2] Fraunhofer ITWM, Kaiserslautern/D

11:40 **Comparison of force fields for the prediction of transport properties of lubricants at extreme conditions**
S. Schmitt[1]; S. Stephan[1]; H. Hasse[1]; [1] TU Kaiserslautern/D

12:00 Lunch break

THERMODYNAMICS

13:10 **Molecular simulation of Brown's characteristic curves**
S. Stephan[1]; [1] Technische Universität Kaiserslautern/D

13:30 **Modelling of dipolar contributions to the Helmholtz energy**
J. Staubach[1]; H. Hasse[1]; S. Stephan[1]; [1] TU Kaiserslautern/D

13:50 **Molecular Dynamics Simulations of Furfural and 5Hydroxymethylfurfural Interaction with Metallic Surfaces in the Electrochemical Hydrogenation Process**
S. Rabet[1]; G. Raabe[1]; [1] TU Braunschweig/D

14:10 Coffee break

PROGRAMME

Friday, 3 March 2023

Room: Franz-Patat-Hörsaal

REACTIONS & BIOLOGY

14:40 **Low-temperature and non-ideal kinetics from reactive molecular dynamics analysis**
W. Kopp[1]; F. Schmalz[1]; L. Krep[1]; C. Huang[1]; K. Leonhard[1]; T. Bakaj[1]; A. Khetan[1]; [1] RWTH Aachen University, Aachen/D

15:00 **Understanding alcohol dehydrogenase catalysis and enzyme-substrate binding in non-conventional reaction media**
J. Bittner[1]; N. Zhang[2]; P. Domínguez de María[3]; I. Smirnova[1]; S. Kara[2]; S. Jakobtorweihen[1]; [1] Hamburg University of Technology, Hamburg/D; [2] Leibniz University Hannover/D; [3] Sustainable Momentum S.L., Las Palmas de Gran Canaria/E

15:20 **Molecular simulation of spike proteins of the SARS-CoV-2 virus at vapor-liquid interfaces**
F. Fleckenstein[1]; S. Stephan[1]; H. Hasse[1]; [1] Technische Universität Kaiserslautern, Kaiserslautern/D

15:40 End of the lecture programme

POSTER

P 01 **Quantum Chemistry on Quantum Computers – Application Oriented Simulations of Metal Organic Frameworks on Current NISQ Devices**
C. Possel[1]; [1] Fraunhofer Institute for Chemical Technology ICT, Pfinztal/D

P 02 **Gaussian process based force field calibration for HFO-1132a**
V. Chheda[1]; G. Raabe[2]; U. Römer[1]; [1] TU Braunschweig, Braunschweig/D; [2] Technische Universität Braunschweig, Braunschweig/D

P 03 **Extending the MolMod database to transferable force fields**
S. Stephan[1]; S. Schmitt[1]; G. Kanagalingam[1]; D. Fröscher[1]; F. Fleckenstein[1]; H. Hasse[1]; [1] TU Kaiserslautern, Kaiserslautern/D

P 04 **Reproducibility of molecular simulation data for transport properties of fluids**
F. Fleckenstein[1]; S. Schmitt[1]; D. Fertig[1]; D. Schaefer[1]; J. Lenhard[1]; S. Stephan[1]; H. Hasse[1]; [1] Technische Universität Kaiserslautern, Kaiserslautern/D

P 05 **Study of Phase Equilibria with Molecular Dynamic Simulations using the Isothermal-Isochoric Integration Method**
T. Markert[1]; M. Fleck[1]; G. Bauer[1]; T. Teh[1]; N. Hansen[1]; J. Groß[1]; [1] Universität Stuttgart, Stuttgart/D

P 06 **Mass transfer through vapor-liquid interfaces of binary mixtures studied by non-stationary molecular dynamics simulations**
V. Braten[1]; D. Schaefer[1]; S. Stephan[1]; H. Hasse[1]; [1] TU Kaiserslautern, Kaiserslautern/D

P 07 **ms2: A molecular dynamics and Monte Carlo simulation engine**
S. Stephan[1]; S. Deublein[1]; B. Eckl[1]; J. Stoll[1]; S. Lishchuk[2]; G. Guevara-Carrion[3]; C. Glass[4]; T. Merker[1]; M. Bernreuther[4]; S. Reiser[1]; G. Rutkai[3]; A. Köster[3]; A. Wafai[4]; M. Horsch[1]; T. Janzen[3]; M. Schappals[1]; M. Kohns[1]; T. Windmann[3]; R. Fingerhut[3]; I. Nitzke[3]; D. Saric[3]; J. Marx[1]; K. Langenbach[1]; D. Celný[5]; H. Hasse[1]; J. Vrabec[3]; [1] TU Kaiserslautern/D; [2] University of Leicester, Leicester/UK; [3] TU Berlin, Berlin/D; [4] High Performance Computing Center Stuttgart, Stuttgart/D; [5] Czech Technical University, Prague/D

P 08 **FAIR research data and epistemic metadata for molecular methods**
M. Horsch[1]; B. Schembera[2]; S. Stephan[3]; [1] Norges miljø- og biovitenskapelige universitet, Ås/N; [2] Universität Stuttgart, Stuttgart/D; [3] TU Kaiserslautern, Kaiserslautern/D

P 09 **Solvation Free Energy Studies of Refrigerant-Lubricant Mixtures**
J. Bode[1]; G. Raabe[1]; [1] TU Braunschweig, Braunschweig/D

P 10 **Solubility and transport properties of light gases in glyceline-water mixtures investigated by molecular dynamics simulations**
M. Spera[1]; J. Range[1]; J. Pleiss[1]; N. Hansen[1]; [1] University of Stuttgart, Stuttgart/D

P 11 **On the dielectric behavior of dipolar model fluids**
M. Kohns[1]; J. Marx[2]; K. Langenbach[2]; [1] TU Kaiserslautern, Kaiserslautern/D; [2] Universität Innsbruck, Innsbruck/A

POSTER

P 12 **Phase Equilibria in Stimuli-Responsive Gels: A PC-SAFT and Molecular Dynamics Study of Smart PNiPAAm Gels**
K. Eckert[1]; [1] Hamburg University of Technology, Hamburg/D

P 13 **Static and dynamic fluid properties in mesoporous confinement**
M. Högler[1]; N. Hansen[1]; H. Kraus[1]; [1] Universität Stuttgart, Stuttgart/D

P 14 **The relation of fluid interfacial properties and the phase diagram**
J. Staubach[1]; S. Stephan[1]; [1] TU Kaiserslautern, Kaiserslautern/D

P 15 **Thermo-Hydrodynamic Density Functional Theory - Non-isothermal Vapor-Liquid Interfaces**
R. Stierle[1]; J. Gross[1]; [1] Universität Stuttgart, Stuttgart/D

P 16 **Entropy Scaling for Inhomogeneous Systems**
B. Bursik[1]; R. Stierle[1]; A. Schlaich[1]; J. Gross[1]; [1] University of Stuttgart, Stuttgart/D

P 17 **Properties of vapor-liquid-liquid interfaces: Predictions by molecular simulation and density gradient theory**
F. Fleckenstein[1]; S. Stephan[1]; [1] Technische Universität Kaiserslautern, Kaiserslautern/D

P 18 **Free energy calculations for the predictions of protein adsorption isotherms**
M. Fiedler[1]; T. Waluga[1]; I. Smirnova[1]; S. Jakobtorweihen[1]; [1] Technische Universität Hamburg, Hamburg/D

P 19 **A molecular dynamics simulation study of the Kapitza heat transfer resistance**
S. Schmitt[1]; S. Stephan[1]; H. Hasse[1]; [1] TU Kaiserslautern, Kaiserslautern/D

P 21 **Prediction of solvation free energies for organometallic compounds via molecular dynamic simulations**
M. Sprick[1]; G. Raabe[1]; [1] Technische Universität Braunschweig, Braunschweig/D

ORGANIZER

DECHEMA e.V.
Theodor-Heuss-Allee 25
60486 Frankfurt am Main
Germany
www.dechema.de

CONTACT

Sabine Urbanczyk
Tel.: +49 69-7564-295
Email: sabine.urbanczyk@dechema.de