Jun. Prof. Dr.-Ing. Maximilian Kohns

Contact Information

Address: RPTU Kaiserslautern*
Erwin-Schrödinger-Str. 44
D-67663 Kaiserslautern
Germany
Phone: +49 631 205 4028
Mail: maximilian.kohns@rptu.de
Web: https://mv.rptu.de/en/dpts/ltd/research/assistant-professorship-electrolyte-thermodynamics-and-molecular-simulation

Personal Information

Birth: 15 May 1990, Neuwied, Germany
Citizenship: German
Family: Married, two sons (born 03/22 and 12/18)

Research Interests

- Electrochemical Systems and Processes
- Chemical Processes with Electrolytes
- Experimental Measurement of Properties of Electrolyte Solutions
- Empirical Modeling of Electrolyte Solutions
- Molecular Modeling and Simulation of Polar Fluids and Electrolyte Solutions
- Multicriteria Optimization

Scientific Career

08/18 – today: Junior Professor for 'Electrolyte Thermodynamics and Molecular Simulation', Department of Mechanical and Process Engineering, RPTU Kaiserslautern

01/18 – 07/18: Postdoctoral Researcher, Molecular Systems Engineering Group (Prof. Amparo Galindo, Prof. George Jackson), Imperial College London, UK

10/17: PhD in Engineering (Dr.-Ing.) with the Thesis:
'Molecular Simulation of Activities in Electrolyte Solutions'
Department of Mechanical and Process Engineering, TU Kaiserslautern
Final Grade: With Distinction

09/13 – 12/17: PhD Student, Scientific Staff, Laboratory of Engineering Thermodynamics (Prof. Hans Hasse), TU Kaiserslautern

Education

04/09 – 08/13: Student of 'Mechanical and Process Engineering', TU Kaiserslautern, Academic Title: Dipl.-Ing. (equivalent to M.Sc.), Final Grade: 1.5

01/13 – 08/13: Diploma's Thesis on 'Molecular Simulation Study of Wetting of Structured Component Surfaces' at the Laboratory of Engineering Thermodynamics (Prof. Hans Hasse), Final Grade: 1.0

07/12 – 10/12: Internship on the Design of Mobile Excavators, Volvo CE, Konz, Germany

* Effective 1 January 2023, the former TU Kaiserslautern changed its name to RPTU Kaiserslautern.

Participation in Boards / Committees

06/21 – today: Speaker of the 'ProcessNet-Nachwuchsgruppe Junges Kollegium Thermodynamik' (Early Career Academic Thermodynamicists)

09/19 – 05/21: Co-Speaker of the 'ProcessNet-Nachwuchsgruppe Junges Kollegium Thermodynamik' (Early Career Academic Thermodynamicists)

10/21 – today: Member of the Council of the Department of Mechanical and Process Engineering, TU Kaiserslautern

Awards

06/18: Award of the 'Freundeskreis der TU Kaiserslautern' (Friends of the TU Kaiserslautern) for an outstanding PhD Thesis

10/13: Award for the best Diploma's Thesis, issued by 'Wissenschaftlicher Arbeitskreis Technische Thermodynamik' (Scientific Working Group of Engineering Thermodynamics in Germany) at the 'Thermodynamik Kolloquium 2013' in Hamburg, Germany

Cooperation

- Prof. Dr. Michael Bortz, Fraunhofer ITWM Kaiserslautern:
  Multicriteria optimization of molecular models
- Prof. Dr.-Ing. Jakob Burger, TU München:
  Thermodynamics of poorly specified electrolyte solutions
- Prof. Dr. Amparo Galindo, Imperial College London:
  Extension of the SAFT-γ Mie Equation of State to electrolyte solutions
- Jun. Prof. Dr.-Ing. Fabian Jirasek, RPTU Kaiserslautern:
  Machine learning of fluid properties based on hybrid data sets
- Prof. Dr.-Ing. Kai Langenbach, Universität Innsbruck:
  Molecular modeling and simulation of polar fluids and their dielectric behavior
- Prof. Dr.-Ing. Heidrun Steinmetz, RPTU Kaiserslautern:
  Recovery of phosphorus from communal wastewater
- Prof. Dr.-Ing. Jadran Vrabec, TU Berlin:
  Development of the molecular simulation tool ms2, permittivity of electrolyte solutions
- Dr.-Ing. Irenäus Wlokas, Universität Duisburg-Essen:
  Development of single droplet models for spray flame synthesis of nanoparticles

Supervised PhD Projects

- Schäfer, Dominik: *Molecular Simulation of Processes at Fluid Interfaces and Electrolyte Solutions (finished 2023)*
- Keller, Alexander: *Thermodynamic Properties of Mixtures for Spray Flame Synthesis of Nanoparticles (finished 2020)*
- Kulkarni, Aditya: *Multicriteria Optimization of Molecular Models of Water (since 2017)*
- Müller, Silvie: *Gas Phase Reactions in Cold Plasma (since 2017)*
- Babette Kunstmann: *Thermodynamic Analysis of the Causes of Micro-Explosions of Droplets in Nanoparticle Synthesis in Spray Flames (since 2020)*
- Heiß, Jana: *Thermodynamics of Electrolyte Solutions for All-Vanadium-Redox-Flow-Batteries (since 2021)*

Lectures

- Thermodynamics II (4 ECTS, Bachelor)
  Summer terms 2019, 2020, 2021, 2022
- Electrolyte Thermodynamics (3 ECTS, Master)
  Winter terms 2018/2019, 2019/2020, 2020/2021, 2021/2022, 2022/2023
- Molecular Thermodynamics (3 ECTS, Bachelor/Master)
  Winter terms 2018/2019, 2019/2020, 2020/2021
- Computer Laboratory on Molecular Simulation (3 ECTS, Master)
  Summer terms 2019, 2020, 2021, 2022, 2023
- Electrochemical Energy Storage (3 ECTS, Master)
  Summer terms 2022, 2023
- Contributions to the 'Seminar TechnoPhysik' (Engineering Physics) (3 ECTS, Bachelor)
  Every term since winter term 2018/2019
- Contribution to collaborative lecture series 'Modern Energy Systems'
  Summer term 2023

Further Teaching-related Activities

- Mentor for students of 'Bio- und Chemieingenieurwissenschaften'
  (Biochemical and Chemical Engineering)
- Supervision of more than 40 student's theses
- Chair of the selection committee of the Clara-Immerwahr- and Gerd-Maurer-Awards
  (excellence award for chemical engineering students at RPTU Kaiserslautern)

Reviewer for

- German Research Foundation (Deutsche Forschungsgemeinschaft, DFG)
- More than a dozen international journals with peer-review
- Alexander von Humboldt-Stiftung (Alexander von Humboldt Foundation)
- Studienstiftung des deutschen Volkes (German Academic Scholarship Foundation)
- Several German High-Performance Computing Centers

Scientific Contributions of Jun. Prof. Dr.-Ing. Maximilian Kohns

Publications in peer-reviewed journals

1. B. Kunstmann, I. Wlokas, **M. Kohns**, H. Hasse: Simulation Study of Superheating in Evaporating Droplets of (TTIP + *p*-Xylene) in Spray Flame Synthesis, *Applications in Energy and Combustion Science* 15 (2023) 100156, DOI: https://doi.org/10.1016/j.jaecs.2023.100156.
2. B. Kunstmann, **M. Kohns**, H. Hasse: Thermophysical Properties of Mixtures of 2-Ethylhexanoic Acid and Ethanol, *J. Chem. Eng. Data* 68 (2023) 330-338, DOI: https://doi.org/10.1021/acs.jced.2c00689.
3. J. Marx, **M. Kohns**, K. Langenbach: Vapor-liquid Equilibria of Binary Mixtures Containing Stockmayer-type Model Fluids from Monte-Carlo Simulations, *Fluid Phase Equilib.* 568 (2023) 113742, DOI: https://doi.org/10.1016/j.fluid.2023.113742.
4. S. Müller, E. Ströfer, **M. Kohns**, K. Münnemann, E. von Harbou, H. Hasse: Investigation of Partial Oxidation of Methane in a Cold Plasma Reactor with Detailed Product Analysis, *Plasma Chem. Plasma Process.* 43 (2023) 513-532, DOI: https://doi.org/10.1007/s11090-022-10308-5.
5. D. Schaefer, **M. Kohns**: Molecular Dynamics Study of Ion Clustering in Concentrated Electrolyte Solutions for the Estimation of Salt Solubilities, *Fluid Phase Equilib.* 571 (2023) 113802, DOI: https://doi.org/10.1016/j.fluid.2023.113802.
6. D. Schaefer, **M. Kohns**, H. Hasse: Molecular Modeling and Simulation of Aqueous Solutions of Alkali Nitrates, *J. Chem. Phys.* 158 (2023) 134508, DOI: https://doi.org/10.1063/5.0141331.
7. E. Baumeister, J. Voggenreiter, **M. Kohns**, J. Burger: Measurement and Modeling of the Solubility of α-Lactose in Water-Ethanol Electrolyte Solutions at 298.15 K, *Fluid Phase Equilib.* 556 (2022) 113378, DOI: https://doi.org/10.1016/j.fluid.2022.113378.
8. A. Keller, J. Burger, H. Steinmetz, H. Hasse, **M. Kohns**: Thermodynamic Modeling of Phosphorus Recovery from Wastewater, *Waste and Biomass Valorization* 13 (2022) 3013-3023, DOI: https://doi.org/10.1007/s12649-022-01700-5.
9. A. Kulkarni, **M. Kohns**, M. Bortz, K.-H. Küfer, H. Hasse: Regularities of Pareto Sets in Low-dimensional Practical Multi-criteria Optimisation Problems: Analysis, Explanation, and Exploitation, *Optimization and Engineering* (2022), DOI: https://doi.org/10.1007/s11081-022-09746-z.
10. J. Marx, **M. Kohns**, K. Langenbach: Systematic Study of Vapour–Liquid Equilibria in Binary Mixtures of Fluids with Different Polarity from Molecular Simulations, Mol. Phys. (2022) e2141150, DOI: https://doi.org/10.1080/00268976.2022.2141150.
11. R. Fingerhut, G. Guevara-Carrion, I. Nitzke, D. Saric, J. Marx, K. Langenbach, S. Prokopev, D. Celný, M. Bernreuther, S. Stephan, **M. Kohns**, H. Hasse, J. Vrabec: *ms2*: A Molecular Simulation Tool for Thermodynamic Properties, Release 4.0, *Comput. Phys. Commun.* 262 (2021) 107860, DOI: https://doi.org/10.1016/j.cpc.2021.107860.
12. A. Keller, J. Burger, H. Hasse, **M. Kohns**: Application of the Pitzer Model for Describing the Evaporation of Seawater, *Desalination* 503 (2021) 114866, DOI: https://doi.org/10.1016/j.desal.2020.114866.
13. A. Keller, I. Wlokas, **M. Kohns**, H. Hasse: Thermophysical Properties of Mixtures of Titanium(IV) Isopropoxide (TTIP) and 2-Propanol (iPOH), *J. Chem. Eng. Data* 66 (2021) 1296-1304, DOI: https://doi.org/10.1021/acs.jced.0c00941.

14. A. Keller, I. Wlokas, **M. Kohns**, H. Hasse: Solid-liquid Equilibria in Mixtures of Iron(III) Nitrate Nonahydrate and Ethanol or 1-Propanol, *Fluid Phase Equilib.* 536 (2021) 112987, DOI: https://doi.org/10.1016/j.fluid.2021.112987.
15. **M. Kohns**, J. Marx, K. Langenbach: Critical Assessment of Perturbation Theories for the Relative Permittivity of Dipolar Model Fluids, *Chem. Eng. Sci.* 245 (2021) 116875, DOI: https://doi.org/10.1016/j.ces.2021.116875.
16. P. Narasu, A. Keller, **M. Kohns**, H. Hasse, E. Gutheil: Numerical Study of the Evaporation and Thermal Decomposition of a Single Iron(III) Nitrate Nonahydrate/Ethanol Droplet, *Int. J. Therm. Sci.* 170 (2021) 107133, DOI: https://doi.org/10.1016/j.ijthermalsci.2021.107133.
17. A. J. Haslam, A. González-Pérez, S. Di Lecce, S. H. Khalit, F. A. Perdomo, S. Kournopoulos, **M. Kohns**, T. Lindeboom, M. Wehbe, S. Febra, G. Jackson, C. S. Adjiman, A. Galindo: Expanding the Applications of the SAFT-γ Mie Group-Contribution Equation of State: Prediction of Thermodynamic Properties and Phase Behavior of Mixtures, *J. Chem. Eng. Data* 65 (2020) 5862-5890, DOI: https://doi.org/10.1021/acs.jced.0c00746.
18. N. Hayer, **M. Kohns**: Thermodynamically Rigorous Description of the Open Circuit Voltage of Redox Flow Batteries, *J. Electrochem. Soc.* 167 (2020) 110516, DOI: https://doi.org/10.1149/1945-7111/ab9e85.
19. A. Keller, I. Wlokas, **M. Kohns**, H. Hasse: Thermophysical Properties of Mixtures of Titanium(IV) Isopropoxide (TTIP) and *p*-Xylene, *J. Chem. Eng. Data* 65 (2020) 869-876, DOI: https://dx.doi.org/10.1021/acs.jced.9b01059.
20. A. Keller, I. Wlokas, **M. Kohns**, H. Hasse: Thermophysical Properties of Solutions of Iron(III) Nitrate Nonahydrate in Mixtures of 1-Propanol and Water, *J. Chem. Eng. Data* 65 (2020) 5413-5420, DOI: https://dx.doi.org/10.1021/acs.jced.0c00531.
21. A. Keller, I. Wlokas, **M. Kohns**, H. Hasse: Thermophysical Properties of Solutions of Iron(III) Nitrate-Nonahydrate in Mixtures of Ethanol and Water, *J. Chem. Eng. Data* 65 (2020) 3519-3527, DOI: https://doi.org/10.1021/acs.jced.0c00105.
22. **M. Kohns**: Molecular Simulation Study of Dielectric Constants of Pure Fluids and Mixtures, *Fluid Phase Equilib.* 506 (2020) 112393, DOI: https://doi.org/10.1016/j.fluid.2019.112393.
23. **M. Kohns**, G. Lazarou, S. Kournopoulos, E. Forte, F. A. Perdomo, G. Jackson, C. S. Adjiman, A. Galindo: Predictive Models for the Phase Behaviour and Solution Properties of Weak Electrolytes: Nitric, Sulfuric and Carbonic Acids, *Phys. Chem. Chem. Phys.* 22 (2020) 15248-15269, DOI: https://doi.org/10.1039/C9CP06795G.
24. **M. Kohns**, J. Marx, K. Langenbach: Relative Permittivity of Stockmayer-Type Model Fluids from MD Simulations and COFFEE, *J. Chem. Eng. Data* 65 (2020) 5891-5896, DOI: https://doi.org/10.1021/acs.jced.0c00769.
25. A. Kulkarni, M. Bortz, K.-H. Küfer, **M. Kohns**, H. Hasse: Multicriteria Optimization of Molecular Models of Water Using a Reduced Units Approach, *J. Chem. Theory Comput.* 16 (2020) 5127-5138, DOI: https://doi.org/10.1021/acs.jctc.0c00301.
26. A. Kulkarni, R. Fingerhut, **M. Kohns**, H. Hasse, J. Vrabec: Correction to "Molecular Modeling and Simulation of Vapor–Liquid Equilibria of Ethylene Oxide, Ethylene Glycol, and Water as Well as their Binary Mixtures", *Ind. Eng. Chem. Res.* 59 (2020) 20232-20234, DOI: https://doi.org/10.1021/acs.iecr.0c04937.
27. A. Kulkarni, E. J. García, A. Damone, M. Schappals, S. Stephan, **M. Kohns**, H. Hasse: A Force Field for Poly(oxymethylene) Dimethyl Ethers (OME*n*), *J. Chem. Theory Comput.* 16 (2020) 2517-2528, DOI: https://dx.doi.org/10.1021/acs.jctc.9b01106.

28. K. Langenbach, **M. Kohns**: Relative Permittivity of Dipolar Model Fluids from Molecular Simulation and from the Co-Oriented Fluid Functional Equation for Electrostatic Interactions, *J. Chem. Eng. Data* 65 (2020) 980-986, DOI: https://doi.org/10.1021/acs.jced.9b00296.
29. K. Langenbach, **M. Kohns**: Correction to "Relative Permittivity of Dipolar Model Fluids from Molecular Simulation and from the Co-Oriented Fluid Functional Equation for Electrostatic Interactions", *J. Chem. Eng. Data* 65 (2020) 5071-5072, DOI: https://dx.doi.org/10.1021/acs.jced.0c00745.
30. P. Narasu, A. Keller, **M. Kohns**, H. Hasse, E. Gutheil: Numerical Study of Single Iron (III) Nitrate Nonahydrate/Ethanol Droplet Evaporation in Humid Air, *Proceedings of the 5th World Congress on Momentum, Heat and Mass Transfer (MHMT'20)* (2020) DOI: https://doi.org/10.11159/icmfht20.183.
31. D. Saric, **M. Kohns**, J. Vrabec: Dielectric Constant and Density of Aqueous Alkali Halide Solutions by Molecular Dynamics: A Force Field Assessment, *J. Chem. Phys.* 152 (2020) 164502, DOI: https://doi.org/10.1063/1.5144991.
32. P. Weingart, P. Hütchen, A. Damone, **M. Kohns**, H. Hasse, W. R. Thiel: Two Simple and Highly Efficient Variants of the Griffith-Ley Oxidation of Alcohols, *ChemCatChem* 12 (2020) 3919-3928, DOI: https://doi.org/10.1002/cctc.202000413.
33. J. Neuhaus, D. Bellaire, **M. Kohns**, E. von Harbou, H. Hasse: Self-Diffusion Coefficients in Solutions of Lithium Bis(fluorosulfonyl)imide with Dimethyl Carbonate and Ethylene Carbonate, *Chem. Ing. Tech.* 91 (2019) 1633-1639, DOI: https://doi.org/10.1002/cite.201900040.
34. **M. Kohns**, M. Horsch, H. Hasse: Partial Molar Volume of NaCl and CsCl in Mixtures of Water and Methanol by Experiment and Molecular Simulation, *Fluid Phase Equilib.* 458 (2018) 30-39, DOI: https://doi.org/10.1016/j.fluid.2017.10.034.
35. S. Becker, **M. Kohns**, H. Urbassek, M. T. Horsch, H. Hasse: Static and Dynamic Wetting Behavior of Drops on Impregnated Structured Walls by Molecular Dynamics Simulation, *J. Phys. Chem. C* 121 (2017) 12669-12683, DOI: https://doi.org/10.1021/acs.jpcc.6b12741.
36. **M. Kohns**, M. T. Horsch, H. Hasse: Activity Coefficients from Molecular Simulations Using the OPAS Method, *J. Chem. Phys.* 147 (2017) 144108, DOI: http://dx.doi.org/10.1063/1.4991498.
37. **M. Kohns**, S. Werth, M. T. Horsch, E. von Harbou, H. Hasse: Molecular Simulation Study of the CO_2-N_2O Analogy, *Fluid Phase Equilib.* 442 (2017) 44-52, DOI: https://doi.org/10.1016/j.fluid.2017.03.007.
38. G. Rutkai, A. Köster, G. Guevara-Carrion, T. Janzen, M. Schappals, C. W. Glass, M. Bernreuther, A. Wafai, S. Stephan, **M. Kohns**, S. Reiser, S. Deublein, M. T. Horsch, H. Hasse, J. Vrabec: *ms2*: A Molecular Simulation Tool for Thermodynamic Properties, Release 3.0, *Comput. Phys. Commun.* 221 (2017) 343-351, DOI: https://doi.org/10.1016/j.cpc.2017.07.025.
39. **M. Kohns**, S. Reiser, M. Horsch, H. Hasse: Solvent Activity in Electrolyte Solutions from Molecular Simulation of the Osmotic Pressure, *J. Chem. Phys.* 144 (2016) 084112, DOI: https://doi.org/10.1063/1.4942500.
40. **M. Kohns**, M. Schappals, M. Horsch, H. Hasse: Activities in Aqueous Solutions of the Alkali Halide Salts from Molecular Simulation, *J. Chem. Eng. Data* 61 (2016) 4068-4076, DOI: https://doi.org/10.1021/acs.jced.6b00544.

41. S. Werth, **M. Kohns**, K. Langenbach, M. Heilig, M. Horsch, H. Hasse: Interfacial and Bulk Properties of Vapor-liquid Equilibria in the System Toluene + Hydrogen Chloride + Carbon Dioxide by Molecular Simulation and Density Gradient Theory + PC-SAFT, *Fluid Phase Equilib.* 427 (2016) 219-230, DOI: https://doi.org/10.1016/j.fluid.2016.07.016.

Invited lectures

1. **M. Kohns**: Thermodynamik von Elektrolytlösungen - von molekularen Grundlagen zu elektrochemischen Anwendungen (Invited Lecture), *Thermodynamik-Kolloquium*, Chemnitz, 26.-28.09.2022.
2. **M. Kohns**: Thermodynamic Modelling of Electrolyte Solutions (Invited Lecture), *Annual Meeting of the Statistical Mechanics and Thermodynamics Group of the Royal Society of Chemistry: "Solving the Electrolyte Problem"*, Manchester, UK, 09.-11.01.2019.

Contributed lectures

1. **M. Kohns**, J. Marx, K. Langenbach: On the Dielectric Behavior of Dipolar Model Fluids, *International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD)*, Tarragona, Spain, 21.-25.05.2023.
2. **M. Kohns**, A. Kulkarni, M. Bortz, K. H. Küfer, H. Hasse: Hierarchical Multi-criteria Optimisation of Molecular Models of Water Using Five Objectives, *International Workshop on Molecular Modeling and Simulation*, Frankfurt, 02.-03.03.2023.
3. J. Marx, **M. Kohns**, K. Langenbach: Co-Oriented Fluid Functional Equation for Electrostatic Interactions (COFFEE) for Mixtures: Phase Behavior and Fluid Structure in Mixtures of Differently Polar Fluids, *AIChE Annual Meeting*, Phoenix, AZ, USA, 13.-18.11.2022.
4. J. Marx, **M. Kohns**, K. Langenbach: Theorie und molekulare Simulation der Dampf-Flüssigkeits-Gleichgewichte von Mischungen verschieden polarer Fluide, *Thermodynamik-Kolloquium*, Chemnitz, 26.-28.09.2022.
5. D. Schaefer, B. Kunstmann, **M. Kohns**, H. Hasse: Characteristics of Droplet Explosions Studied with Non-Equilibrium Molecular Dynamics Simulations, *AIChE Annual Meeting*, Phoenix, AZ, USA, 13.-18.11.2022.
6. D. Schaefer, B. Kunstmann, **M. Kohns**, H. Hasse: Characteristics of Droplet Explosions Studied with Non-Equilibrium Molecular Dynamics Simulations, *(Bio)Process Engineering - a Key to Sustainable Development*, Aachen, 12.-15.09.2022.
7. J. Marx, **M. Kohns**, K. Langenbach: Phase Equilibria in Mixtures of Differently Polar Fluids: Molecular Simulation and Perturbation Theory, *(Bio)Process Engineering - a Key to Sustainable Development*, Aachen, 12.-15.09.2022.
8. **M. Kohns**, J. Marx, K. Langenbach: Dielectric Properties of Model Fluids from Molecular Dynamics and Perturbation Theories, *Thermodynamics*, Bath, UK, 07.-09.09.2022.
9. J. Marx, **M. Kohns**, K. Langenbach: Vapor Liquid Equilibria of Mixtures of Fluids with Different Polarity, *32nd European Symposium of Applied Thermodynamics (ESAT)*, Graz, Austria, 17.-20.07.2022.
10. E. Baumeister, **M. Kohns**, J. Burger: Measurement and Modeling of the Solubility of α-Lactose in Water-Ethanol Electrolyte Solutions, *Thermodynamik-Kolloquium*, Web-Conference, 27.-29.09.2021.
11. A. Kulkarni, M. Bortz, K.-H. Küfer, **M. Kohns**, H. Hasse: Multi-criteria Optimisation of Molecular Models of Water Using the Reduced Units Method, *Thermodynamik-Kolloquium*, Web-Conference, 27.-29.09.2021.

12. A. Kulkarni, M. Bortz, K.-H. Küfer, **M. Kohns**, H. Hasse: Multi-criteria Optimisation of Molecular Models of Water, *Twenty-first Symposium on Thermophysical Properties*, Web-Conference, 20.-26.06.2021.
13. **M. Kohns**, J. Marx, K. Langenbach: Molecular Thermodynamics Approach to the Relative Permittivity, *Twenty-first Symposium on Thermophysical Properties*, Web-Conference, 20.-25.06.2021.
14. E. Baumeister, **M. Kohns**, J. Burger: Modeling Phase Equilibria of Poorly Specified Mixtures Using a Perturbation Term, *13th European Congress of Chemical Engineering (ECCE) and 6th European Congress of Applied Biotechnology (ECAB)*, Web-Conference, 20.-23.09.2021.
15. S. Müller, **M. Kohns**, E. Ströfer, H. Hasse: Reaction Engineering Studies of a Cold Plasma Reactor, *13th European Congress of Chemical Engineering (ECCE) and 6th European Congress of Applied Biotechnology (ECAB)*, Web-Conference, 20.-23.09.2021.
16. S. Müller, **M. Kohns**, E. Ströfer, H. Hasse: A Cold Plasma Reactor for Partial Oxidation of Methane, *International Congress of Chemical and Process Engineering (CHISA)*, Web-Conference, 15.-18.03.2021.
17. **M. Kohns**, S. Kournopoulos, S. di Lecce, G. Lazarou, E. Forte, F. A. Perdomo, G. Jackson, C. S. Adjiman, A. Galindo: Modelling Aqueous Solutions of Strong and Weak Electrolytes with the SAFT-γ Mie Equation of State, *6th SAFT Symposium (Joint Event with 31st European Symposium on Applied Thermodynamics (ESAT))*, Web-Conference, 05.-09.07.2021.
18. K. Langenbach, **M. Kohns**: Thermodynamic and Dielectric Properties from an Equation of State, *6th SAFT Symposium (Joint Event with 31st European Symposium on Applied Thermodynamics (ESAT))*, Web-Conference, 05.-09.07.2021.
19. **M. Kohns**, J. Marx, K. Langenbach: Molecular Thermodynamics Approach to the Relative Permittivity, *International Workshop on Molecular Modeling and Simulation*, Web-Conference, 01.-02.03.2021.
20. A. M. Kulkarni, M. Bortz, K.-H. Küfer, **M. Kohns**, H. Hasse: Multi-criteria Optimisation of Molecular Models of Water, *International Workshop on Molecular Modeling and Simulation*, Web-Conference, 01.-02.03.2021.
21. **M. Kohns**, A. Keller, I. Wlokas, H. Hasse: Thermophysical Properties and Reactions in Precursor Solutions for the Production of Nanoparticles, *4th International Symposium Gas-Phase Synthesis of Functional Nanomaterials: Fundamental Understanding, Modeling and Simulation, Diagnostics, Scale-up and Application*, Web-Conference, 6.10.-09.10.2020.
22. A. Keller, J. Burger, **M. Kohns**, H. Steinmetz, H. Hasse: Thermodynamische Modellierung und Prozesssimulation der Phosphorrückgewinnung aus Abwasser, *Jahrestreffen der ProcessNet-Fachgruppen Fluidverfahrenstechnik und Membrantechnik*, Potsdam, 27.-29.03.2019.
23. **M. Kohns**, S. Kournopoulos, S. di Lecce, G. Lazarou, E. Forte, F. A. Perdomo Hurtado, G. Jackson, C. S. Adjiman, A. Galindo: Modelling Electrolyte Solutions with the SAFT-γ Mie Equation of State, *Thermodynamik-Kolloquium*, Duisburg, 30.09.-02.10.2019.
24. A. Keller, J. Burger, **M. Kohns**, H. Steinmetz, H. Hasse: Thermodynamische Modellierung und Prozesssimulation der Phosphorrückgewinnung aus Abwasser, *ProcessNet Jahrestreffen*, Aachen, 10.-13.09.2018.
25. M. Heier, S. Becker, F. Diewald, **M. Kohns**, M. Horsch, R. Müller, H. Hasse: Modeling and Simulation of Wetting of Component Surfaces, *International Workshop on Molecular Modeling and Simulation*, Frankfurt, 09.-10.03.2017.

26. M. Heier, S. Becker, F. Diewald, **M. Kohns**, M. Horsch, R. Müller, H. Hasse: Modeling and Simulation of Wetting of Component Surfaces, *European Symposium on Applied Thermodynamics (ESAT)*, Bucharest, Romania, 18.-21.05.2017.
27. **M. Kohns**, M. Schappals, M. Horsch, H. Hasse: Molecular Simulation of Activities in Electrolyte Solutions, *International Workshop on Molecular Modelling and Simulation*, Frankfurt, 09.-10.03.2017.
28. **M. Kohns**, M. Schappals, M. Horsch, H. Hasse: Molecular Simulation of Activities in Electrolyte Solutions, *European Symposium on Applied Thermodynamics (ESAT)*, Bucharest, Romania, 18.-21.05.2017.
29. **M. Kohns**, M. Schappals, M. Horsch, H. Hasse: Molecular Simulation of Activities in Electrolyte Solutions, *Thermodynamics*, Edinburgh, UK, 05.-09.09.2017.
30. M. Horsch, **M. Kohns**, S. Reiser, H. Hasse: Solvent Activity in Electrolyte Solutions by Molecular Simulation of the Osmotic Pressure, *Physics of Liquid Matter: Modern Problems (PLMMP)*, Kiev, Ukraine, 27.-31.03.2016.
31. M. Horsch, **M. Kohns**, S. Reiser, M. Schappals, H. Hasse: Activities in Electrolyte Solutions by Molecular Simulation of the Osmotic Pressure, *American Institute of Chemical Engineers (AIChE) Annual Meeting*, San Francisco, CA, USA, 13.-18.11.2016.
32. **M. Kohns**, S. Reiser, M. Horsch, H. Hasse: Molekulare Simulation von Aktivitäten in Elektrolytlösungen, *Thermodynamik-Kolloquium*, Kaiserslautern, 05.-07.10.2016.
33. S. Becker, **M. Kohns**, M. Horsch, H. Hasse: Molecular Modeling and Simulation of Wetting of Solid Surfaces, *Thermodynamics*, Copenhagen, Denmark, 15.-18.09.2015.
34. **M. Kohns**, S. Reiser, M. Horsch, H. Hasse: Molecular Simulation of Organic Electrolyte Solutions, *American Institute of Chemical Engineers (AIChE) Annual Meeting*, Salt Lake City, UT, USA, 08.-13.11.2015.
35. **M. Kohns**, E. von Harbou, M. Horsch, H. Hasse: Molecular Simulation Study of the CO_2-N_2O Analogy, *European Symposium on Applied Thermodynamics (ESAT)*, Athens, Greece, 11.-14.06.2015.
36. S. Reiser, **M. Kohns**, M. Horsch, H. Hasse: Molecular Simulation of Organic Electrolyte Solutions, *International Workshop on Molecular Modeling and Simulation*, Frankfurt, 23.-24.03.2015.
37. M. Horsch, S. Becker, **M. Kohns**, S. Werth, H. Hasse: Molecular Modelling and Simulation of Adsorption and Wetting of Structured Surfaces, *Collaborative Computational Project 5 (CCP5) Annual Meeting*, Telford, Great Britain, 10.09.2014.
38. M. Horsch, S. Becker, **M. Kohns**, S. Werth, H. Hasse: Molekulare Simulation von realen Fluiden an Phasengrenzflächen, *Jahrestreffen der ProcessNet-Fachgemeinschaft für Fluiddynamik und Trenntechnik (FDTT)*, Würzburg, 27.09.2013.
39. M. T. Horsch, S. Becker, **M. Kohns**, X. Rozanska, S. Werth, H. Hasse: Molecular Modelling of Adsorption on Real Component Surfaces, *MedeA Users Group Meeting*, Wien, Österreich, 19.09.2013.

Poster presentations

1. **M. Kohns**, J. Marx, K. Langenbach: On the Dielectric Behavior of Dipolar Model Fluids (Poster), *International Workshop on Molecular Modeling and Simulation*, Frankfurt, 02.-03.03.2023.

2. J. Marx, **M. Kohns**, K. Langenbach: Prediction of Molecular Orientations and Phase Equilibria of Mixtures with the Co-Oriented Fluid Functional Equation for Electrostatic Interactions (COFFEE) (Poster), *International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD)*, Tarragona, Spain, 21.-25.05.2023.
3. B. Kunstmann, **M. Kohns**, H. Hasse: Phase Equilibria of Solvent Mixtures for Spray Flame Synthesis of Nanomaterials (Poster), *Thermodynamik-Kolloquium*, Chemnitz, 26.-28.09.2022.
4. S. Mross, D. Bellaire, **M. Kohns**, K. Münnemann, H. Hasse: Self-diffusion Coefficients in Mixtures of OME with Alkanes (Poster), *Thermodynamik-Kolloquium*, Chemnitz, 26.-28.09.2022.
5. P. Zittlau, **M. Kohns**, F. Jirasek: Prediction of the Density of Electrolyte Solutions with Matrix Completion Methods (Poster), *Thermodynamik-Kolloquium*, Chemnitz, 26.-28.09.2022.
6. D. Schaefer, **M. Kohns**, H. Hasse: Molecular Modeling and Simulation of Aqueous Solutions of Alkali Nitrate Salts (Poster), *(Bio)Process Engineering - a Key to Sustainable Development*, Aachen, 12.-15.09.2022.
7. D. Schaefer, **M. Kohns**, H. Hasse: A Set of Molecular Models for Alkali Nitrates in Aqueous Solution (Poster), *Thermodynamics*, Bath, UK, 07.-09.09.2022.
8. **M. Kohns**, J. Marx, K. Langenbach: Fundamentals of the Dielectric Behavior of Polar Fluids from Molecular Dynamics Simulations (Poster), *Foundations of Molecular Modeling and Simulation (FOMMS) 2022: Molecular Modeling and the Data Revolution*, Delavan, WI, USA, 17.-21.07.2022.
9. N. Hayer, **M. Kohns**: Thermodynamically Rigorous Description of the Open Circuit Voltage of Redox Flow Batteries (Poster), *Thermodynamik-Kolloquium*, Web-Conference, 27.-29.09.2021.
10. B. Kunstmann, **M. Kohns**, H. Hasse: Thermodynamic Properties of Solvent Mixtures for Spray Flame Synthesis of Nanomaterials: 2-Ethylhexanoic Acid (EHA) + (Ethanol / p-Xylene) (Poster), *Thermodynamik-Kolloquium*, Web-Conference, 27.-29.09.2021.
11. D. Schaefer, **M. Kohns**, H. Hasse: Molecular Modeling and Simulation of Aqueous Solutions of Alkali Nitrate Salts (Poster), *Thermodynamik-Kolloquium*, Web-Conference, 27.-29.09.2021.
12. A. Kulkarni, E. J. Garcia, A. Damone, S. Stephan, M. Schappals, **M. Kohns**, H. Hasse: A Molecular Model for Poly(oxymethylene) Dimethyl Ethers (Poster), *Twenty-First Symposium on Thermophysical Properties*, Web-Conference, 20.-26.06.2021.
13. **M. Kohns**, S. Kournopoulos, S. Di Lecce, G. Lazarou, E. Forte, F. A. Perdomo, G. Jackson, C. S. Adjiman, A. Galindo: Predictive Models for the Phase Behaviour and Solution Properties of Weak Electrolytes: Nitric, Sulfuric and Carbonic Acids (Poster), *Twenty-first Symposium on Thermophysical Properties*, Web-Conference, 20.-25.06.2021.
14. N. Hayer, **M. Kohns**: Thermodynamically Rigorous Description of the Open Circuit Voltage of Redox Flow Batteries (Poster), *Annual Meeting on Reaction Engineering, Web-Conference*, 10.-12.05.2021.
15. S. Müller, **M. Kohns**, E. Ströfer, H. Hasse: Partial Oxidation of Methane in a Cold Plasma Reactor (Poster), *Annual Meeting on Reaction Engineering*, Web-Conference, 10.-12.05.2021.
16. **M. Kohns**: Molecular Simulation Study of the Relative Permittivity of Pure Fluids and Mixtures (Poster), *31st European Symposium on Applied Thermodynamics (ESAT)*, Web-Conference, 05.-09.07.2021.

17. A. Kulkarni, M. Bortz, K. H. Küfer, **M. Kohns**, H. Hasse: Multi-criteria Optimisation of Molecular Models of Water Using the Reduced Units Method (Poster), *31st European Symposium on Applied Thermodynamics (ESAT)*, Web-Conference, 05.-09.07.2021.
18. A. Kulkarni, E. J. Garcia, A. Damone, S. Stephan, M. Schappals, **M. Kohns**, H. Hasse: A Force Field for Poly(oxymethylene) Dimethyl Ethers (Poster), *31st European Symposium on Applied Thermodynamics (ESAT)*, Web-Conference, 05.-09.07.2021.
19. **M. Kohns**, S. Kournopoulos, S. Di Lecce, G. Lazarou, E. Forte, F. A. Perdomo Hurtado, G. Jackson, C. S. Adjiman, A. Galindo: Predictive Models for the Phase Behaviour and Solution Properties of Weak Electrolytes: Nitric, Sulfuric and Carbonic Acids (Poster), *International Workshop on Molecular Modeling and Simulation*, Web-Conference, 01.-02.03.2021.
20. A. M. Kulkarni, E. J. Garcia, A. Damone, S. Stephan, M. Schappals, **M. Kohns**, H. Hasse: A Molecular Model for Poly(oxymethylene) Dimethyl Ethers (Poster), *International Workshop on Molecular Modeling and Simulation*, Web-Conference, 01.-02.03.2021.
21. A. M. Kulkarni, M. Bortz, K.-H. Küfer, **M. Kohns**, H. Hasse: Multi-criteria Optimisation and Dimensionless Quantities: Applications in Thermodynamics (Poster), *Indo-German Workshop on Advances in Materials, Reaction and Separation Processes*, Berlin, 23.02-26.02.2020.
22. S. Müller, **M. Kohns**, E. Ströfer, H. Hasse: Gas Phase Reactions of Methane and Oxygen in Cold Plasma (Poster), *ProcessNet-Jahrestagung und DECHEMA-Jahrestagung der Biotechnologen*, Web-Conference, 21.-24.09.2020.
23. **M. Kohns**, G. Lazarou, E. Forte, F. A. Perdomo Hurtado, G. Jackson, C. S. Adjiman, A. Galindo: Thermodynamic Modelling of Weak Electrolytes Using the SAFT-γ Mie Equation of State (Poster), *International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD)*, Vancouver, Canada, 12.-16.05.2019.
24. **M. Kohns**, G. Lazarou, E. Forte, F. A. Perdomo Hurtado, G. Jackson, C. S. Adjiman, A. Galindo: Thermodynamic Modelling of Weak Electrolytes Using the SAFT-γ Mie Equation of State (Poster), *Thermodynamics*, Huelva, Spain, 26.-28.06.2019.
25. A. M. Kulkarni, E. Garcia, A. Damone, S. Stephan, M. Schappals, **M. Kohns**, H. Hasse: A Transferable Force Field for Poly(oxymethylene) Dimethyl Ethers (Poster), *Thermodynamik-Kolloquium*, Duisburg, 30.09.-02.10.2019.
26. A. M. Kulkarni, **M. Kohns**, M. Bortz, H. Hasse: Pareto Optimisation of Molecular Models of Water using a Reduced Units Approach (Poster), *Thermodynamik-Kolloquium*, Duisburg, 30.09.-02.10.2019.
27. A. M. Kulkarni, E. Garcia, S. Stephan, A. Damone, **M. Kohns**, H. Hasse: A Transferable Force Field for Poly(oxymethylene) Dimethyl Ethers (Poster), *Thermodynamik-Kolloquium*, Kassel, 26.-28.09.2018.
28. **M. Kohns**, M. Horsch, H. Hasse: Molecular Simulation Study of Dielectric Constants of Pure Fluids and Mixtures (Poster), *Thermodynamik-Kolloquium*, Dresden, 27.-29.09.2017.
29. S. Becker, M. Heier, **M. Kohns**, M. Horsch, H. Hasse: Contact Angle of Droplets on Nanostructured Surfaces by Molecular Simulation (Poster), *Thermodynamik-Kolloquium*, Kaiserslautern, 05.-07.10.2016.
30. **M. Kohns**, S. Reiser, M. Horsch, H. Hasse: Solvent Activity in Electrolyte Solutions from Molecular Simulation of the Osmotic Pressure (Poster), *International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD)*, Porto, Portugal, 22.-26.05.2016.

31. **M. Kohns**, E. von Harbou, M. Horsch, H. Hasse: Molecular Modelling of Nitrous Oxide and its Application in the CO_2-N_2O Analogy (Poster), *International Workshop on Molecular Modeling and Simulation*, Frankfurt, 23.-24.03.2015.
32. **M. Kohns**, E. von Harbou, M. Horsch, H. Hasse: Molecular Simulation Study of the CO_2-N_2O Analogy (Poster), *Thermodynamics*, Copenhagen, Denmark, 15.-18.09.2015.
33. **M. Kohns**, E. von Harbou, M. Horsch, H. Hasse: Molecular Simulation Study of the CO_2-N_2O Analogy (Poster), *Thermodynamik-Kolloquium*, Bochum 05.-07.10.2015.
34. S. Becker, **M. Kohns**, M. Horsch, H. Hasse: Wettability of Rough Solid Surfaces: A Molecular Simulation Study (Poster), *WE-Heraeus-Seminar "Wetting of Structures with Complex Geometries"*, Physikzentrum Bad Honnef, 16.-19.03.2014.
35. **M. Kohns**, M. Horsch, H. Hasse: Molecular Modelling of Nitrous Oxide and its Application in the CO_2-N_2O Analogy (Poster), *Thermodynamik-Kolloquium*, Stuttgart, 22.-24.09.2014.
36. S. Becker, **M. Kohns**, M. Horsch, H. Hasse: Wettability of Rough Solid Surfaces: A Molecular Simulation Study (Poster), *Thermodynamik-Kolloquium*, Hamburg, 07.-09.10.2013.
37. **M. Kohns**, S. Becker, M. Horsch, H. Hasse: Molekulare Simulation der Benetzung geometrisch rauer Oberflächen (Poster), *Thermodynamik-Kolloquium*, Hamburg, 07.-09.10.2013.