List of Publications

Books

G. Raabe**,** *Molecular Simulation Studies on Thermophysical Properties – with Application to Working Fluids*, Springer Series „Molecular Modeling and Simulation: Applications and Perspectives“ (2017).

Peer Reviewed Publications in International Journals (h-index = 21)

- J. Schilke, M. Sprick, E. Schneider, J. A. Ledezma Fierro, A. Pradald , G. Raabe, A. Schallmey, Efficient lignin dissolution and enzymatic depolymerization in ethylene glycol-based deep eutectic solvent mixtures: Integrated experimental and molecular dynamics study. *J. Phys. Chem. B* (2026) DOI: 10.1021/acs.jpcb.5c07451
- A. Kale, G. Raabe, Developing Interface Force Fields for Water and Oxygen on Pt, and Pt_3Ni, Pt_3Co alloy surfaces for Proton Exchange Membrane Fuel Cell (PEMFC) applications, *ACS Omega* (2026), DOI: 10.1021/acsomega.5c11427
- G. Raabe, Viral P. Chheda, U.Römer, Sequential Bayesian Force Field Calibration of Lennard-Jones Parameters with Experimental Data. *I&ECR* (2025), DOI: 10.1021/acs.iecr.5c00708
- S. Ringe, G. Raabe, Atomistic simulations of heterogeneous electrocatalysis at the center of sustainable carbon feedstocks. *Current Opinion in Electrochemistry* 51, 101671 (2025) DOI: 10.1016/j.coelec.2025.101671
- G. Raabe, Predictive Molecular Simulation Studies on the VaporLiquid Equilibria of Ten Binary Mixtures Containing Different Hydrofluoroolefins. *J. Chem. Eng. Data* 69 (11), p.3999-4010, DOI: 10.1021/acs.jced.4c00464 (2024)
- S. Okeil, S. Rabet, G. Valadez Huerta, G. Raabe, G. Garnweitner: Understanding the Role of Solvent on the Growth of Zinc Oxide: Insight from Experiment and Molecular Dynamics Simulations. *Langmuir* DOI 10.1021/acs.langmuir.4c00921 (2024).
- S. Rabet, W. Tobaschus, G. Chung, T Gimpel, G. Raabe, D. Schröder, B. Munirathinam: Exploring Impurity Effects and Catalyst Surface Features in Furfural Electroreduction for Jet Fuel Precursor Production: Experimental and Molecular Dynamics Insights. *ChemElectroChem* (2024) DOI: 10.1002/celc.202400336
- M. Sprick, G. Raabe, Prediction of Toluene/Water Partition Coefficients of SAMPL9 compounds: Comparison of the molecular dynamics force fields GAFF/RESP and GAFF/IPolQ-Mod+LJ-fit, *Physical Chemistry Chemical Physics* 26, 3126-3138 (2024), DOI: 10.1039/D3CP04149B
- J. Bode, G.Raabe, Molecular dynamics studies of the solubility behavior of carbon dioxide (CO2), difluoromethane (R-32), 1-chloro-3,3,3-trifluoropropene (R-1233zd(E)) and 2,3,3,3-tetrafluoro-1-propene (R-1234yf) in pentaerythritol tetra(2-ethylhexanoate) (PEB8), pentaerythritol tetrabutyrate (PEC4) and pentaerythritol tetraoctanoate (PEC8). *J. Comput. Chem*. doi.org/10.1002/jcc.27196 (2023).
- T. Lenk, S. Rabet, M. Sprick, G. Raabe, U. Schröder, Insight into the interaction of furfural with metallic surfaces in the electrochemical hydrogenation process. *ChemPhysChem* DOI**:** 10.1002/cphc.202200614 (2022).
- S. Rabet. G. Raabe, Comparison of the GAFF, OPLSAA and CHARMM27 Force fields for the reproduction of the Thermodynamics Properties of Furfural, 2-Methylfuran, 2,5-Dimethylfuran and 5-Hydroxymethylfuran. *Fluid Phase Equil*. 554, 113331, DOI: 10.1016/j.fluid.2021.113331 (2021).
- G. Valadez-Huerta; G. Raabe, Genetic Parameterization of Interfacial Force Fields based on Classical Bulk Force Fields and Ab initio Data: Application to the Methanol-ZnO Interfaces. *J. Chem. Inf. Model*. 60, 6033-6043, https://doi.org/10.1021/acs.jcim.0c01093 (2020)
- A. Mecklenfeld, G. Raabe, GAFF/IPolQ-Mod+LJ-Fit: Optimized Force Field Parameters for Solvation Free Energy Predictions. *ADMET & DMPK* 8 (3), 274-296 DOI: 10.5599/admet.837 (Special Issue. Strategies of solubility enhancement and perspectives in solubility measurements of pharmaceutical compounds (2020).
- G. Raabe, Purely Predictive Vapor-Liquid-Equilibrium Properties of 3,3,4,4,4-pentafluoro-1-butene (HFO-1345fz), 2,3,3,4,4,4-hexafluoro-1-butene (HFO-1336yf) and trans-1-chloro-2,3,3,3-tetrafluoropropene (HCFO-1224yd(E)) from Molecular Simulation, *J. Chem. Eng. Data* (Invited contribution to the *Special Issue*)

- A. Mecklenfeld, G. Raabe, Applicability of a Thermodynamic Cycle Approach for a Force Fields Parametrization Targeting Non-Aqueous Solvation Free Energies. *J. Computer-Aided Molecular Design (JCAM)* 34 (1), 71-82*,* DOI: 10.1007/s10822-019-00261-5 (2020).
- G. Raabe, Parameterization Approach for a Systematic Extension of the HFO Force Field to Fluorinated Butenes and HCFO Compounds. *J. Chem. Eng. Data* 65(3), 1234-1242 (2020) DOI 10.1021/acs.jced.9b00588 (Invited contribution to the *Special Issue in Honour of Professor Hans Hasse*).
- G. Raabe, M.G. Hopkins, C. C. Sampson, P. L. Stanwix, E. F. May, Dielectric properties of binary hydrofluoroolefin refrigerant mixtures: Comparisons of new experimental data with molecular dynamics simulations. *J. Chem. Thermodynamics* 10.1016/j.jct.2019.105985 (2019).
- G. Raabe, Molecular Simulation Studies on Refrigerants, Past-Present-Future. *Fluid Phase Equilibria 485, 190-198.* doi: 10.1016/j.fluid.2018.12.022 (2019) (Invited contribution to the *Special Issue*: *Molecular Simulation*).
- G. Raabe, Molecular Simulation Studies on the Vapor-Liquid Phase Equilibria of Binary Mixtures of HFO-1123 with R-32, R-1234yf, R-1234ze(E), R-134a and CO_2 and their Modelling by the PCP-SAFT Equation of State, Data in brief 25, 104014, https://doi.org/10.1016/j.dib.2019.104014 (associated with the FPE paper) (2019)
- A. Mecklenfeld and G. Raabe, Comparison of RESP and IPolQ-Mod Partial Charges for Solvation Free Energy Calculations of Various Solute/Solvent Pairs. *J. Chem. Theory Comput., 13 (12) 6266-6274,* DOI: 10.1021/acs.jctc.7b00692, (2017).
- M. Schappals, A. Mecklenfeld, L. Kröger, V. Botan, A. Köster, S. Stephan, E. J. Garcias, G. Rutkai, G. Raabe, P. Klein, K. Leonhard, C. W. Glass, J. Lenhard, J. Vrabec and H. Hasse, Round Robin Study: Molecular Simulation of Thermodynamic Properties from Models with Internal Degrees of Freedom. *J. Chem. Theory Comput*. 13, 4270-4280, DOI: 10.1021/acs.jctc.7b00489, (2017).
- A. Mecklenfeld and G. Raabe, Efficient Solvation Free Energy Simulations: Impact of Soft-Core Potential and a New Adaptive λ-Spacing Method. *Mol. Phys*. 115, 1322-1334 (2017). *Data* (Invited contribution to the *Special Issue in Honour of Professor Johann Fischer*).
- G. Raabe, Molecular simulation studies on HFO working fluids and their blends. *STBE* 22 (8), 1077-1089 (2016). (Invited contribution to the STBE special issue: *Low GWP Working Fluids*.)
- P. Petr and G. Raabe, Evaluation of R-1234ze(Z) as drop-in replacement for R-245fa in Organic Rankine Cycles - From thermophysical properties to cycle performance. *Energy* 93, 266-274 (2015).
- G. Raabe, Molecular Simulation Studies on the Vapor-Liquid-Equilibria of the cis- and trans-HCFO-1233zd, and the cis- and trans-HFO-1336mzz. *J. Chem. Eng. Data* 60 (8), 2412-2419 (2015). http://dx.doi.org/10.1021/acs.jced.5b00286
- C. Schulze, G. Raabe, W. J. Tegethoff and J. Köhler, Transient Evaluation of a City Bus Air Conditioning System with R-445A as Drop-In - From the Molecules to the System. *Int. J. Therm. Sci*. 96, 335-361 (2015).
- G. Raabe, Molecular Dynamics Studies on Liquid Phase Dynamics and Structures of Four Different Fluoropropenes and their Binary Mixtures with R-32 and CO_2. *J. Phys. Chem. B* 118 (1), 240-254 (2014).
- G. Raabe, Molecular Simulation Studies on the Thermophysical Properties of the Refrigerant Blend R-445A. *J. Chem. Eng. Data* 58, 3470-3476 (2013).
- G. Raabe, Molecular Simulation Studies on the Vapor-Liquid Phase Equilibria of Binary Mixtures of R-1234yf and R-1234ze(E) with R-32 and CO_2. *J. Chem. Eng. Data* 58 (6), 1867-1873 (2013).
- G. Raabe and R. J. Sadus, Molecular dynamics simulation of the effect of bond flexibility on the transport properties of water. *J. Chem. Phys*. 127, 104701 (2012).
- G. Raabe, Molecular Modeling of Fluoropropene Refrigerants. *J. Phys. Chem. B.* 116, 5744-5751 (2012).
- G. Raabe and R. J. Sadus, Molecular dynamics simulation of the dielectric constant of water: the effect of bond flexibility. *J. Chem. Phys.* 134, 234501 (2011).
- N. Anh Lai, J. Vrabec, G. Raabe, J. Fischer and M. Wendland, Description of HFO-1234yf with BACKONE equation of state. *Fluid Phase Equilibria* 305, 204-211 (2011).
- G. Raabe and E. J. Maginn, A Force Field for 3,3,3-fluoro-1-propenes, including HFO-1234yf. *J. Phys. Chem. B.* 114, 10133-10142 (2010).

- G. Raabe and E. J. Maginn, Molecular Modeling of the Vapor-Liquid Equilibrium Properties of the Alternative Refrigerant 2,3,3,3-Tetrafluoro-1-propene (HFO-1234yf). *J. Phys. Chem. Lett.* 1, 93-96 (2010). Correction. *J. Phys. Chem. Lett.* 1, 2675 (2010).
- G. Raabe and J. Köhler, Thermodynamical and structural properties of binary mixtures of imidazolium chloride ionic liquids and alcohols from molecular simulation. *J. Chem. Phys*. 129, 144503 (2008).
- G. Raabe and J. Köhler, Thermodynamical and structural properties of imidazolium based ionic liquids from molecular simulation; *J. Chem. Phys*. 128, 154509 (2008).
- J. Janisch, G. Raabe and J. Köhler, Vapor-Liquid Equilibria and Saturated Liquid Densities in Binary Mixtures of Nitrogen, Methane, and Ethane and Their Correlation Using the VTPR and PSRK GCEOS ; *J. Chem. Eng. Data*; 52, 1897-1903 (2007).
- G. Raabe and R. J. Sadus, Influence of bond flexibility on the vapor-liquid phase equilibria of water. *J. Chem. Phys.* 126, 044701 (2007).
- G. Raabe, B. D. Todd and R. J. Sadus, Molecular simulation of the shear viscosity and the self-diffusion coefficient of mercury along the vapor-liquid coexistence curve. *J. Chem. Phys.* 123, 034511 (2005).
- G. Raabe and J. Köhler, Phase equilibria in the system nitrogen-ethane and their prediction using cubic equation of state with different types of mixing rules. *Fluid Phase Equilibria* 222-223, 3-9 (2004).
- G. Raabe and R. J. Sadus, Molecular Simulation of the Vapor-Liquid Coexistence of Mercury. *J. Chem. Phys*. 119 (3), 6691-6697 (2003).
- G. Raabe and J. Köhler, Use of ab initio interaction energies for the prediction of phase equilibria in the system nitrogen-ethane. *Phys. Chem. Chem. Phys*. 4, 926-930 (2002).
- G. Raabe, J. Janisch and J. Köhler, Experimental studies of phase equilibria in mixtures relevant for the description of natural gases. *Fluid Phase Equilibria*, 185 (1-2), 199-208 (2001).

Invited Lectures

- G. Raabe, Molecular simulation and its application to HFO working fluids. *HYDROGENIUS – I^2CNER Joint Research Symposium, I^2CNER Annual Symposium*, *Kyushu University Energy Week*, Fukuoka, Japan (2017).

Conference Contributions and Proceedings

- L. Schnelting, B. G. Bederna, G. Raabe, U. Römer, C. Thomas, Bayesian Calibration of HEOS Mixing Models and Impact Thermodynamic Cycles. Paper ID 7470*, Conference Proceedings ECOS,* Paris, Frankreich 2025 . DOI: 10.26434/chemrxiv-2025-vnm16.
- L. Schnelting, U. Römer, and G. Raabe. Boundary-Constrained Gaussian Processes for the Calculation Of Vapor-Liquid-Equilibrium Surfaces. *UNCECOMP 2025*, 15–18, Rhodes, Greece. 2025.
- A. Kale, G. Raabe, Optimizing Interface Force Fields for water on platinum (111). *International Workshop on Molecular Modeling and Simulation*, Frankfurt (2025).
- M. Sprick, E. Schneider, W. Dann, G. Raabe, Molecular characterization of organic materials for redox-flow batteries. *International Workshop on Molecular Modeling and Simulation*, Frankfurt (2025).
- E. Schneider, M. Sprick, C. Matke, G. Raabe, Development of methodologies for a rational design of enzymatic catalytic reaction cascade. Poster presentation, *International Workshop on Molecular Modeling and Simulation*, Frankfurt (2025).
- G. Raabe, New parametrization approach for molecular models, and predictive simulation studies on refrigerant blends and refrigerant-lubricant mixtures. *22nd Symposium on Thermophysical Properties*, Boulder, USA (2024).
- S. Rabet, G. Raabe. Molecular Dynamics Simulations of Furfural and 5-Hydroxymethylfurfural interaction with metallic surfaces in the electrochemical hydrogenation process. *International Workshop on Molecular Modeling and Simulation*, Frankfurt (2023).
- M. Sprick, G. Raabe, Prediction of solvation free energies for organometallic compounds via molecular dynamics simulations. Poster presentation, *International Workshop on Molecular Modeling and Simulation*, Frankfurt (2023).
- V. P. Chheda, G. Raabe, U. Römer, Gaussian process based force field calibration for HFO-1132a. Poster presentation*, International Workshop on Molecular Modeling and Simulation*, Frankfurt (2023).

- J. Bode, G. Raabe, Solvation free energy studies of refrigerant-lubricant mixtures. Poster presentation, *International Workshop on Molecular Modeling and Simulation*, Frankfurt (2023).
- J. Pudack, J.-P. Mai and G.Raabe, Investigation of a Novel Process for the Production of Silicon via the Selective Condensation of Silicon Monoxide, *Proceeding of the Silicon for the Chemical & Solar Industry XVI* (2022) ISBN 978-82-692919-0-2, http://dx.doi.org/10.2139/ssrn.4125102.
- G. Raabe, Molecular modelling and simulation studies for various HFO and HCFO compounds and their mixtures, *21th Symposium on Thermophysical Properties, Online Conference* (2021).
- S. Rabet, M. Sprick, A. Mecklenfeld and G. Raabe, Investigation of Electrochemical Synthesis of 2-Methylfuran from Furfural by Molecular Dynamics Simulation. *ProcessNet-Jahrestreffen Molekulare Modellierung und Simulation,* online (2021).
- A. Mecklenfeld and G. Raabe, Solvation Free Energy Predictions from Molecular Dynamics Simulations by Improved Alchemical Pathways and optimized Force Fields Parameters. *3rd International Symposium on Pharmaceutical Engineering Research- SPhERe*, Braunschweig, Deutschland (2019).
- A. Mecklenfeld and G. Raabe, Comparison of RESP and IPolQ-Mod Partial Charges by Efficient Molecular Simulations of Free Energy of Solvation. *20th Symposium on Thermophysical Properties*, Boulder, USA (2018).
- G. Raabe, Molecular Modeling and Simulation Studies o HFO and HCFO Based Working Fluids. *20th Symposium on Thermophysical Properties*, Boulder, USA (2018).
- A. Mecklenfeld and G. Raabe, Efficient molecular simulations of the free energy of solvation. *ProcessNet-Biennial Meeting Molecular Modeling and Simulation,* Frankfurt, Germany (2017)
- G. Raabe, A Force Field for HFO Working Fluids and its Application to Simulation Studies on HFO-1123. *4th International Conference on Molecular Simulation (ICMS),* Shanghai, China (2016)
- A. Mecklenfeld and G. Raabe, Improving Alchemical Pathway for Free Energy Calculations. *4th International Conference on Molecular Simulation (ICMS),* Shanghai, China (2016)
- A. Mecklenfeld and G. Raabe, Einfluss von Simulations- und Evaluationsmethoden auf die Berechnung der freien Enthalpiedifferenz der Solvatisierung. *Thermodynamik-Kolloquium,* Kaiserslautern, Germany (2016).
- A. Mecklenfeld and G. Raabe, Predicting the solubility of drug candidates. *Symposium on Pharmaceutical Engineering Research*, Braunschweig, Germany (2015).
- G. Raabe, Molecular simulation studies on HFO based working fluids. *19th Symposium on Thermophysical Properties,* Boulder, USA (2015).
- G. Raabe, Molecular simulation studies on HFO working fluids and their blends. *Intern. Workshop Molecular Modeling and Simulation,* Frankfurt, Germany (2015).
- J.-P. Mai and G. Raabe, High-purity Silicon from Pellets using Direct Carbothermic Reduction in a Microwave Furnace. *29th European Photovoltaic Solar Energy Conference and Exhibition,* Amsterdam, The Netherlands (2014).
- J.-P. Mai and G. Raabe, Tracing impurities in silicon production in the microwave furnace. *143nd Annual Meeting & Exhibition, TMS 2014,* San Diego, USA (2014), as well as 4th Int. Conf. on Crystalline Silicon Photovoltaics, s-Hertogenbosch, The Netherlands (2014).
- J. Köhler, G. Raabe, C. Schulze and W. J. Tegethoff, Transient Simulation of a City Bus Air Conditioning System with R-445A as Drop-In Starting from Molecular Simulation. *International Colloquium 150th Birthday of Richard Mollier,* Dresden, Germany (2013).
- J. Köhler, G. Raabe, C. Schulze and W. J. Tegethoff, Transient Simulation of Mobile R-445A Air Conditioning Systems – From the Molecules to the System. *SAE-International,* Troy, USA (2013).
- G. Raabe, Molecular simulation studies on the thermophysical properties of fluoropropenes refrigerants and their mixtures. *2nd Rostock Symposium on Thermophysical Properties for Technical Thermodynamic*, Rostock, Germany (2013).
- J.-P. Mai, G. Raabe and J. Köhler, On the reaction mechanisms of carbothermal silicon production; reactive Molecular Dynamics Studies. *142nd Annual Meeting & Exhibition, TMS 2013,* San Antonio, USA (2013).
- G. Raabe, Molecular simulation studies on fluoropropenes refrigerants and blends. *Intern. Workshop Molecular Modeling and Simulation: Natural Science meets Engineering*, Frankfurt, Deutschland (2013).
- J.-P. Mai and G. Raabe, Molecular simulation studies on the role of gaseous intermediates in silicon production using the reactive force field ReaxFF-lg. *Intern. Workshop Molecular Modeling and Simulation: Natural Science meets Engineering*, Frankfurt, Germany (2013).

- J.-P. Mai, G. Raabe and J. Köhler, Experimental Studies on the Reaction Temperature of Silicon Production in a Microwave Furnace. *27th European Photovoltaic Solar Energy Conference and Exhibition,* Frankfurt, Germany (2012).
- G. Raabe, Molecular Simulation Studies on Alternative Fluoropropene Refrigerants. *18th Symposium on Thermophysical Properties*, Boulder, USA (2012).
- J.-P. Mai, G. Raabe and J. Köhler, Molecular Dynamics Simulation Studies on the SiO_2-C Reaction System using the ReaxFF Reactive Force Field. *18th Symposium on Thermophysical Properties* in Boulder, USA (2012).
- J.-P. Mai, G. Raabe and J. Köhler, Experimental and Molecular Simulation Studies of Silicon Production in a Microwave Furnace. *Silicon for the Chemical and Solar Industry XI*, Bergen, Norway (2012).
- J.-P. Mai, G. Raabe and J. Köhler, Silicon Production in a Microwave Furnace, Experimental and Molecular Studies. *TMS 141th Annual Meeting & Exhibition*, Orlando, USA (2012).
- J.-P. Mai, G. Raabe and J. Köhler, Molecular dynamics Studies on the Reaction System of Silicon Production using the ReaxFF Reactive Force Field. *SimMolMod*, Dortmund, Germany (2011).
- G. Raabe and E. J. Maginn, Molecular modeling of alternative fluoropropene refrigerants, including HFO-1234yf. *Thermodynamics 2011,* Athens, Greece (2011).
- G. Raabe and J. Köhler, Modeling of the thermophysical properties of CO_2-lubricant oil mixtures. *European Conference on Thermophysical Properties*, Thessaloniki, Greece (2011).
- G. Raabe and R. J. Sadus, Bond Flexibility in Water and the Prediction of Thermo-Physical Properties; *AIChE Annual Meeting*, Salt Lake City, USA (2010).
- J.-P. Mai, G. Raabe and J. Köhler, Production of MG-Si with microwave heating. *Silicon for the Chemical and Solar Industry X*, Alesand, Norway (2010).
- G. Raabe and E. J. Maginn, A force field for fluoropropenes, including HFO-1234yf. *Molecular Modelling and Simulation for Industrial Applications: Physico-Chemical Properties and Processes*, Würzburg, Germany (2010).
- G. Raabe and R. J. Sadus, Influence of Bond Flexibility on the Thermophysical Properties of Water. *17th Symposium on Thermophysical Properties*, Boulder, USA (2009).
- G. Raabe and J. Köhler, Molecular Simulation Studies on the Structural Properties of Imidazolium-based Liquids and Solutes. *17th Symposium on Thermophysical Properties* in Boulder, USA (2009).
- G. Raabe and J. Köhler, Bestimmung thermodynamischer und struktureller Eigenschaften ionischer Fluide und ihrer Gemische mittels Molekularer Simulation. *GVC Thermodynamik-Kolloquium*, Erlangen, Germany (2008).
- G. Raabe and R. J. Sadus, Influence of bond flexibility on the vapor-liquid phase equilibria of water. *20th International Conference on Chemical Thermodynamics ICCT*, Warsaw, Poland (2008).
- G. Raabe and J. Köhler, Molecular Simulation Studies on the Structural Properties of Imidazolium-based Ionic Liquids and their binary Mixtures with Alcohols. *20th International Conference on Chemical Thermodynamics ICCT*, Warsaw, Poland (2008).
- G. Raabe and J. Köhler, Thermodynamische and strukturelle Eigenschaften ionischer Fluide aus Molekularer Simulation. *GVC Thermodynamik-Kolloquium*, Rostock, Germany (2007).
- G. Raabe and J. Köhler, PVT-Properties of Mixtures of Imidazolium based Ionic Liquids and Alcohols from Molecular Simulation. *16th Symposium on Thermophysical Properties*, Boulder, USA (2006).
- S. Bröcker, M. Kleiber, G. Raabe and M. Schiller, Alternativen zu NRTL, UNIQUAC and UNIFAC für industrielle Anwendungen. *GVC Thermodynamik-Kolloquium* in Wittenberg, Deutschland (2004).
- G. Raabe and R. J. Sadus, Molecular Simulation of the Vapor-Liquid Coexistence of Mercury. *20th ESAT,* Lahnstein, Germany; Preprints*:* P093*,* 473-476 (2003).
- G. Raabe and J. Köhler, Phase equilibria in the system nitrogen-ethane and their prediction using cubic equations of state with different types of mixing rules. *15th Symposium on Thermophysical Properties* in Boulder, USA; paper p706.pdf (2003).
- G. Raabe and J. Köhler, Use of ab initio interaction energies for NRTL to predict phase equilibria in the system nitrogen-ethane. *15th Symposium on Thermophysical Properties*, Boulder, USA (2003).

- G. Raabe and J. Köhler, Use of ab initio interaction energies for the prediction of phase equilibria in the system nitrogen-ethane. *International Bunsen Discussion Meeting: Global Phase Diagrams*, Walberberg, Germany (2001).
- G. Raabe, J. Janisch and J. Köhler, Experimental Studies of Phase Equilibria in Systems of Natural Gas. *14th Symposium on Thermophysical Properties*, Boulder, USA; paper NAT03RAA.PDF (2000).

Final Reports of Research Projects

- G. Raabe*, Systematic extension of a force field for fluorinated propenes to HCFO and longer-chained HFO compounds, and its application for studies on new working fluids*. DFG Funding RA 946/3-1 (2022).
- J.-P. Mai, G. Raabe, *Solarfähiges Silizium aus dem Mikrowellenofen (solar capable silicon from a microwave furnace*) DBU-Entwicklungsprojekt Az-28408
- A. Schröder and G. Raabe, *CO_2-Hochtemperaturwärmepumpe großer Leistung mit Ejektor*, Teilvorhaben (IfT): *Auslegung und Optimierung des Ejektors, Kreislaufsimulationen (CO_2-high temperature high performance heat pump with ejector, Sub-project: Construction and optimisation of the ejector, system simulations),* BMWI joined project 03ET1097B.
- Ch. Kaiser, A. Schröder and G. Raabe, *Entwicklung eines CO_2-Ejektorkreislaufs für eine umschaltbare Wärmepumpen-Klimaanlage für Omnibusklimaanlagen*. *(Development of a CO_2-ejectorcycle for a reversible heat pump-air conditioning system for buses)*. DBU development project Az-30270 (2015).
- G. Raabe, J.-P. Mai and J. Köhler, *Herstellung von Rohsilizium (mg-Si) im Mikrowellenofen (mgSiMiO) (Production of metallurgical silicon in a microwave furnace).* DBU development project, Az-28408 (2013).
- G. Raabe, J. Köhler and M. Sonnekalb, *Untersuchung eines CO_2-Ejektorskreislaufs für Omnibusklimaanlagen (Studies on a CO_2-ejectorcycle for mobile air conditioning systems in buses)*. DBU development project, Az-27385 (2011). http://www.dbu.de/ab/DBU-Abschlussbericht-AZ-27385.pdf
- G. Raabe, *Development of force field models for alternative refrigerants based on fluoropropenes, including HFO-1234yf.* DFG-Fellowship RA 946/2-1 (2010).

Theses

G. Raabe**,** *Molecular Simulation Studies on Thermophysical Properties – with Application to Working Fluids*, Habilitation thesis, Faculty of Mechanical Engineering, TU Braunschweig, Germany (2016); published as monograph in the Springer Series „Molecular Modeling and Simulation: Applications and Perspectives“ (2017).

G. Raabe, *Dampf-Flüssig-Phasengleichgewichte bei tiefen Temperaturen (Vapour-Liquid Equilibria at low Temperatures)*; PhD Thesis, Shaker Aachen, ISBN 3-8322-0717-1 (2002).