

## Veröffentlichungen

### Bücher

G. Raabe, Molecular Simulation Studies on Thermophysical Properties – with Application to Working Fluids, Springer Buchreihe „*Molecular Modeling and Simulation: Applications and Perspectives*”, Springer Nature Singapur ISBN 978-981-10-3544-9 (2017).

### Beiträge in Zeitschriften (h-index = 20, <https://orcid.org/0000-0003-2758-9460>)

- 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 (CO<sub>2</sub>), 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 Equilibria* 554, 11333, 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 (12), 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, https://doi.org/10.5599/admet.837 (2020) (*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* 65 (9), 4318-4325, https://doi.org/10.1021/acs.jced.0c00325 (2020) (Eingeladener Beitrag zum *Special Issue: Alternative Refrigerants*).
- 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 (Eingeladener Beitrag zu einem *Special Issue* zum 60. Geburtstag von 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* 142, 105985, 10.1016/j.jct.2019.105985, 2020.
- 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<sub>2</sub> and their Modelling by the PCP-SAFT Equation of State, *Data in brief* 25, 104014, https://doi.org/10.1016/j.dib.2019.104014 (assoziiert mit FPE Artikel) (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) (Eingeladener Beitrag zum *Special Issue: Molecular Simulation*).
- A. Mecklenfeld und 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), 6266-6272. DOI: 10.1021/acs.jctc.7b00692 (2017).

- M. Schappals, A. Mecklenfeld, L. Kröger, V. Botan, A. Köster, S. Stephan, E. J. Garcias, G. Rutkais, G. Raabe, P. Klein, K. Leonhard, C. W. Glass, J. Lenhard, J. Vrabec und 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 und G. Raabe, Efficient Solvation Free Energy Simulations: Impact of Soft-Core Potential and a New Adaptive  $\lambda$ -Spacing Method. *Mol. Phys.* 115, 1322 (2017). (Eingeladener Beitrag zum *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, DOI:10.1080/23744731.2016.1206796 (2016). (Eingeladener Beitrag zum *STBE Special Issue: Low GWP Working Fluids*).
- P. Petr und 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. <http://dx.doi.org/10.1021/acs.jced.5b00286>, *J. Chem. Eng. Data* 60 (8), 2412-2419 (2015).
- C. Schulze, G. Raabe, W. J. Tegethoff und 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<sub>2</sub>. *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<sub>2</sub>. *J. Chem. Eng. Data* 58 (6), 1867-1873 (2013).
- G. Raabe und 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 und 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 und M. Wendland, Description of HFO-1234yf with BACKONE equation of state. *Fluid Phase Equilibria* 305, 204-211 (2011).
- G. Raabe und 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 und 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 und 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 und J. Köhler, Thermodynamical and structural properties of imidazolium based ionic liquids from molecular simulation; *J. Chem. Phys.* 128, 154509 (2008).
- J. Janisch, G. Raabe und 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 und 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 und 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 und 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 und R. J. Sadus, Molecular Simulation of the Vapor-Liquid Coexistence of Mercury. *J. Chem. Phys.* 119 (3), 6691-6697 (2003).

- G. Raabe und 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 und 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).

#### Eingeladene Vorträge

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

#### Beiträge auf Konferenzen

- 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. Posterpräsentation, 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. Posterpräsentation, International Workshop on Molecular Modeling and Simulation, Frankfurt (2023).
- J. Bode, G. Raabe, Solvation free energy studies of refrigerant-lubricant mixtures. Posterpräsentation, International Workshop on Molecular Modeling and Simulation, Frankfurt (2023).
- J. Pudack, J.-P. Mai und 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, 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 und G. Raabe, Solvation Free Energy Predictions from Molecular Dynamics Simulations by Improved Alchemical Pathways and optimized Force Fields Parameters. *3<sup>rd</sup> International Symposium on Pharmaceutical Engineering Research- SPheRe*, Braunschweig, Deutschland (2019).
- A. Mecklenfeld und G. Raabe, Comparison of RESP and IPolQ-Mod Partial Charges by Efficient Molecular Simulations of Free Energy of Solvation. *20<sup>th</sup> Symposium on Thermophysical Properties*, Boulder, USA (2018).
- G. Raabe, Molecular Modeling and Simulation Studies on HFO and HCFO Based Working Fluids. *20<sup>th</sup> Symposium on Thermophysical Properties*, Boulder, USA (2018).
- A. Mecklenfeld und G. Raabe, Efficient molecular simulations of the free energy of solvation. *ProcessNet-Jahrestreffen Molekulare Modellierung und Simulation*, Frankfurt, Deutschland (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 und G. Raabe, Improving Alchemical Pathway for Free Energy Calculations. *4th International Conference on Molecular Simulation (ICMS)*, Shanghai, China (2016).
- A. Mecklenfeld und G. Raabe, Einfluss von Simulations- und Evaluationsmethoden auf die Berechnung der freien Enthalpiedifferenz der Solvatisierung. *Thermodynamik-Kolloquium*, Kaiserslautern, Deutschland (2016).
- A. Mecklenfeld und G. Raabe, Predicting the solubility of drug candidates. *Symposium on Pharmaceutical Engineering Research*, Braunschweig, Deutschland (2015).
- G. Raabe, Molecular simulation studies on HFO based working fluids. *19<sup>th</sup> 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, Deutschland (2015).

- J.-P. Mai und G. Raabe, High-purity Silicon from Pellets using Direct Carbothermic reduction in a Microwave Furnace. *29<sup>th</sup> European Photovoltaic Solar Energy Conference and Exhibition*, Amsterdam, Niederlande (2014).
- J.-P. Mai und G. Raabe, Tracing impurities in silicon production in the microwave furnace. *143<sup>nd</sup> Annual Meeting & Exhibition, TMS 2014*, San Diego, USA (2014), sowie *4<sup>th</sup> Int. Conf. on Crystalline Silicon Photovoltaics*, Hertogenbosch, Niederlande (2014).
- J. Köhler, G. Raabe, C. Schulze und 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, Deutschland (2013).
- J. Köhler, G. Raabe, C. Schulze und 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. *2<sup>nd</sup> Rostock Symposium on Thermophysical Properties for Technical Thermodynamic*, Rostock, Deutschland (2013).
- J.-P. Mai, G. Raabe und J. Köhler, On the reaction mechanisms of carbothermal silicon production; reactive Molecular Dynamics Studies. *142<sup>nd</sup> 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 und G. Raabe, Molecular simulation studies on the role of gaseous intermediates in silicon production using the reactive force field ReaxFF-Ig. *Intern. Workshop Molecular Modeling and Simulation: Natural Science meets Engineering*, Frankfurt, Deutschland (2013).
- J.-P. Mai, G. Raabe und J. Köhler, Experimental Studies on the Reaction Temperature of Silicon Production in a Microwave Furnace. *27<sup>th</sup> European Photovoltaic Solar Energy Conference and Exhibition*, Frankfurt, Deutschland (2012).
- G. Raabe, Molecular Simulation Studies on Alternative Fluoropropene Refrigerants. *18th Symposium on Thermophysical Properties*, Boulder, USA (2012).
- J.-P. Mai, G. Raabe und J. Köhler, Molecular Dynamics Simulation Studies on the SiO<sub>2</sub>-C Reaction System using the ReaxFF Reactive Force Field. *18th Symposium on Thermophysical Properties* in Boulder, USA (2012).
- J.-P. Mai, G. Raabe und J. Köhler, Experimental and Molecular Simulation Studies of Silicon Production in a Microwave Furnace. *Silicon for the Chemical and Solar Industry XI*, Bergen, Norwegen (2012).
- J.-P. Mai, G. Raabe und J. Köhler, Silicon Production in a Microwave Furnace, Experimental and Molecular Studies. *TMS 141<sup>th</sup> Annual Meeting & Exhibition*, Orlando, USA (2012).
- J.-P. Mai, G. Raabe und J. Köhler, Molecular Dynamics Studies on the Reaction System of Silicon Production using the ReaxFF Reactive Force Field. *SimMolMod 2011*, Dortmund, Deutschland (2011).
- G. Raabe und E. J. Maginn, Molecular modeling of alternative fluoropropene refrigerants, including HFO-1234yf. *Thermodynamics 2011*, Athen, Griechenland (2011).
- G. Raabe und J. Köhler, Modeling of the thermophysical properties of CO<sub>2</sub>-lubricant oil mixtures. *European Conference on Thermophysical Properties*, Thessaloniki, Griechenland (2011).
- G. Raabe und 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 und J. Köhler, Production of MG-Si with microwave heating. *Silicon for the Chemical and Solar Industry X*, Alesund, Norwegen (2010).
- G. Raabe und E. J. Maginn, A force field for fluoropropenes, including HFO-1234yf. *Molecular Modelling and Simulation for Industrial Applications: Physico-Chemical Properties and Processes*, Würzburg, Deutschland (2010).
- G. Raabe und R. J. Sadus, Influence of Bond Flexibility on the Thermophysical Properties of Water. *17th Symposium on Thermophysical Properties*, Boulder, USA (2009).
- G. Raabe und J. Köhler, Molecular Simulation Studies on the Structural Properties of Imidazolium-based Ionic Liquids and Solutes. *17th Symposium on Thermophysical Properties*, Boulder, USA (2009).

- G. Raabe und J. Köhler, Bestimmung thermodynamischer und struktureller Eigenschaften ionischer Fluide und ihrer Gemische mittels Molekularer Simulation. *GVC Thermodynamik-Kolloquium*, Erlangen, Deutschland (2008).
- G. Raabe und R. J. Sadus, Influence of bond flexibility on the vapor-liquid phase equilibria of water. *20th International Conference on Chemical Thermodynamics ICCT*, Warschau, Polen (2008).
- G. Raabe und 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*, Warschau, Polen (2008).
- G. Raabe und J. Köhler, Thermodynamische und strukturelle Eigenschaften ionischer Fluide aus Molekularer Simulation. *GVC Thermodynamik-Kolloquium*, Rostock, Deutschland (2007).
- G. Raabe und 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 und M. Schiller, Alternativen zu NRTL, UNIQUAC und UNIFAC für industrielle Anwendungen. *GVC Thermodynamik-Kolloquium* in Wittenberg, Deutschland (2004).
- G. Raabe und R. J. Sadus, Molecular Simulation of the Vapor-Liquid Coexistence of Mercury. *20th ESAT*, Lahnstein, Deutschland; Preprints: P093, 473-476 (2003).
- G. Raabe und 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*, Boulder, USA; Paper p706.pdf (2003).
- G. Raabe und J. Köhler, Use of ab initio interaction energies for NRTL to predict phase equilibria in the system nitrogen-ethane. *15th Symposium on Thermophysical Properties* in Boulder, USA (2003).
- G. Raabe und 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, Deutschland (2001).
- G. Raabe, J. Janisch und J. Köhler, Experimental Studies of Phase Equilibria in Systems of Natural Gas. *14th Symposium on Thermophysical Properties*, Boulder, USA; Paper NAT03RAA.PDF (2000).

#### Abschlussberichte, Technical reports

- G. Raabe, Systematische Erweiterung eines Force Fields für Fluoropropene auf HCFO und langkettige HFO, und Anwendung zur Untersuchung neuartiger Arbeitsfluide. DFG-Förderprojekt RA946/3-1 (2022).
- G. Valadez-Huerta, G. Raabe, Genetischer Algorithmus zur Entwicklung von Interfacial Force Fields für ZnO Oberflächen, *HLRN Rechenkontingent nic00051* (2020).
- A. Mecklenfeld, G. Raabe, Ansätze zur Beschreibung von Grenzaktivitätskoeffizienten, *HLRN Rechenkontingent nic00060* (2020).
- A. Mecklenfeld, G. Raabe, Molekulare Simulationen zur Vorhersage relativer Löslichkeiten, *HLRN Rechenkontingent nic00025* (2020).
- A. Mecklenfeld, G. Raabe, Predicting the solubility of drug candidates, Project 1C, *MWK Graduate program „μ-Props, Processing of poorly soluble drugs at small scale“* (2019).
- J.-P. Mai, G. Raabe, Solarfähiges Silizium aus dem Mikrowellenofen, *DBU-Entwicklungsprojekt Az-28408* (2017).
- A. Schröder, G. Raabe, J. Köhler, CO<sub>2</sub>-Hochtemperaturwärmepumpe großer Leistung mit Ejektor, *BMW Förderprojekt 03ET1097* (2016).
- Ch. Kaiser, A. Schröder, G. Raabe, Entwicklung eines CO<sub>2</sub>-Ejektorkreislaufs für eine umschaltbare Wärmepumpen-Klimaanlage für Omnibusklimaanlagen. *DBU-Entwicklungsprojekt Az-30270* (2015).
- G. Raabe, J.-P. Mai, J. Köhler, Herstellung von Rohsilizium (mg-Si) im Mikrowellenofen (mgSiMiO). *DBU-Entwicklungsprojekt, Az-28408* (2013).
- G. Raabe, J. Köhler, M. Sonnekalb, Untersuchung eines CO<sub>2</sub>-Ejektorkreislaufs für Omnibusklimaanlagen. *DBU-Entwicklungsprojekt, 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-Stipendium RA 946/2-1* (2010).

**Veröffentlichungen der Dissertation**

G. Raabe, Dampf-Flüssig-Phasengleichgewichte bei tiefen Temperaturen (Dissertation); *Shaker Aachen*, ISBN 3-8322-0717-1 (2002).