Gabriele Raabe

List of Publications by Year in Descending Order

38 papers	836 citations	18 h-index	28 g-index
39 ext. papers	925 ext. citations	3.5 avg, IF	5.14 L-index

#	Paper	IF	Citations
38	Comparison of the GAFF, OPLSAA and CHARMM27 force field for the reproduction of the thermodynamics properties of furfural, 2-methylfuran, 2,5-dimethylfuran and 5-hydroxymethylfurfural. *Fluid Phase Equilibria*, **2022**, 554, 113331	2.5	0
37	Genetic Parameterization of Interfacial Force Fields Based on Classical Bulk Force Fields and Ab Initio Data: Application to the Methanol-ZnO Interfaces. *Journal of Chemical Information and Modeling*, **2020**, 60, 6033-6043	6.1	4
36	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. *Journal of Chemical & Engineering Data*, **2020**, 65, 4318-4325	2.8	4
35	GAFF/IPolQ-Mod+LJ-Fit: Optimized force field parameters for solvation free energy predictions.. *ADMET and DMPK*, **2020**, 8, 274-296	1.3	1
34	Applicability of a thermodynamic cycle approach for a force field parametrization targeting non-aqueous solvation free energies. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 71-82	4.2	1
33	Dielectric properties of binary hydrofluoroolefin refrigerant mixtures: Comparisons of new experimental data with molecular dynamics simulations. *Journal of Chemical Thermodynamics*, **2020** , 142, 105985	2.9	1
32	Parameterization Approach for a Systematic Extension of the Hydrofluoroolefin Force Field to Fluorinated Butenes and Hydrochlorofluoroolefin Compounds. *Journal of Chemical & Engineering Data*, **2020**, 65, 1234-1242	2.8	5
31	Molecular simulation data for the vapor-liquid phase equilibria of binary mixtures of HFO-1123 with R-32, R-1234yf, R-1234ze(E), R-134a and CO and their modelling by the PCP-SAFT equation of state. *Data in Brief*, **2019**, 25, 104014	1.2	1
30	Molecular simulation studies on refrigerants past □present □future. *Fluid Phase Equilibria*, **2019**, 485, 190-198	2.5	17
29	Molecular Models (Force Fields). *Molecular Modeling and Simulation*, **2017**, 145-189		
28	Molecular Simulation Studies on Thermophysical Properties. *Molecular Modeling and Simulation*, **2017**,		11
27	Efficient solvation free energy simulations: impact of soft-core potential and a new adaptive □spacing method. *Molecular Physics*, **2017**, 115, 1322-1334	1.7	8
26	Round Robin Study: Molecular Simulation of Thermodynamic Properties from Models with Internal Degrees of Freedom. *Journal of Chemical Theory and Computation*, **2017**, 13, 4270-4280	6.4	32
25	Comparison of RESP and IPolQ-Mod Partial Charges for Solvation Free Energy Calculations of Various Solute/Solvent Pairs. *Journal of Chemical Theory and Computation*, **2017**, 13, 6266-6274	6.4	12
24	Monte Carlo Simulations. *Molecular Modeling and Simulation*, **2017**, 31-82		1
23	Applications of Molecular Simulations to Studies on Working Fluids. *Molecular Modeling and Simulation*, **2017**, 257-289		1
22	Thermophysical and Structural Properties from Molecular Simulation. *Molecular Modeling and Simulation*, **2017**, 191-256		

21	Molecular simulation studies in hydrofluoroolefine (HFO) working fluids and their blends. *Science and Technology for the Built Environment*, **2016**, 22, 1077-1089	1.8	24
20	Transient evaluation of a city bus air conditioning system with R-445A as drop-in – From the molecules to the system. *International Journal of Thermal Sciences*, **2015**, 96, 355-361	4.1	8
19	Molecular Simulation Studies on the Vapor–Liquid Equilibria of the cis- and trans-HCFO-1233zd and the cis- and trans-HFO-1336mzz. *Journal of Chemical & Engineering Data*, **2015**, 60, 2412-2419	2.8	36
18	Evaluation of R-1234ze(Z) as drop-in replacement for R-245fa in Organic Rankine Cycles – From thermophysical properties to cycle performance. *Energy*, **2015**, 93, 266-274	7.9	39
17	Molecular dynamics studies on liquid-phase dynamics and structures of four different fluoropropenes and their binary mixtures with R-32 and CO2. *Journal of Physical Chemistry B*, **2014**, 118, 240-54	3.4	22
16	Molecular Simulation Studies on the Vapor–Liquid Phase Equilibria of Binary Mixtures of R-1234yf and R-1234ze(E) with R-32 and CO2. *Journal of Chemical & Engineering Data*, **2013**, 58, 1867-1873	2.8	68
15	Molecular Simulation Studies on the Thermophysical Properties of the Refrigerant Blend R-445A. *Journal of Chemical & Engineering Data*, **2013**, 58, 3470-3476	2.8	20
14	Molecular modeling of fluoropropene refrigerants. *Journal of Physical Chemistry B*, **2012**, 116, 5744-51	3.4	49
13	Molecular dynamics simulation of the effect of bond flexibility on the transport properties of water. *Journal of Chemical Physics*, **2012**, 137, 104512	3.9	47
12	Description of HFO-1234yf with BACKONE equation of state. *Fluid Phase Equilibria*, **2011**, 305, 204-211	2.5	26
11	Molecular dynamics simulation of the dielectric constant of water: the effect of bond flexibility. *Journal of Chemical Physics*, **2011**, 134, 234501	3.9	70
10	Molecular Modeling of the Vapor–Liquid Equilibrium Properties of the Alternative Refrigerant 2,3,3,3-Tetrafluoro-1-propene (HFO-1234yf). *Journal of Physical Chemistry Letters*, **2010**, 1, 93-96	6.4	40
9	A force field for 3,3,3-fluoro-1-propenes, including HFO-1234yf. *Journal of Physical Chemistry B*, **2010**, 114, 10133-42	3.4	62
8	Thermodynamical and structural properties of imidazolium based ionic liquids from molecular simulation. *Journal of Chemical Physics*, **2008**, 128, 154509	3.9	56
7	Thermodynamical and structural properties of binary mixtures of imidazolium chloride ionic liquids and alcohols from molecular simulation. *Journal of Chemical Physics*, **2008**, 129, 144503	3.9	34
6	Influence of bond flexibility on the vapor-liquid phase equilibria of water. *Journal of Chemical Physics*, **2007**, 126, 044701	3.9	40
5	Molecular simulation of the shear viscosity and the self-diffusion coefficient of mercury along the vapor-liquid coexistence curve. *Journal of Chemical Physics*, **2005**, 123, 34511	3.9	9
4	Phase equilibria in the system nitrogen–ethane and their prediction using cubic equations of state with different types of mixing rules. *Fluid Phase Equilibria*, **2004**, 222-223, 3-9	2.5	13

3	Molecular simulation of the vapor–liquid coexistence of mercury. *Journal of Chemical Physics*, **2003**, 119, 6691-6697	3.9	41
2	Use of ab initio interaction energies for the prediction of phase equilibria in the system nitrogen–ethane. *Physical Chemistry Chemical Physics*, **2002**, 4, 926-930	3.6	6
1	Experimental studies of phase equilibria in mixtures relevant for the description of natural gases. *Fluid Phase Equilibria*, **2001**, 185, 199-208	2.5	27