Andreas Klamt

List of Publications by Year in Descending Order

119 papers	16,607 citations	46 h-index	124 g-index
124 ext. papers	18,629 ext. citations	3.9 avg, IF	7.05 L-index

#	Paper	IF	Citations
119	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. *Journal of Chemical Physics*, **2021**, 155, 084801	3.9	115
118	COSMO Mechanistic Prediction of Passive Membrane Permeability for Neutral Compounds and Ions and Its pH Dependence. *Journal of Physical Chemistry B*, **2020**, 124, 3343-3354	3.4	11
117	COSMO-RS based predictions for the SAMPL6 logP challenge. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 385-392	4.2	17
116	DRUG SOLUBILITY, REACTION THERMODYNAMICS, AND CO-CRYSTAL SCREENING **2019**, 467-491		2
115	COSMOplex: self-consistent simulation of self-organizing inhomogeneous systems based on COSMO-RS. *Physical Chemistry Chemical Physics*, **2019**, 21, 9225-9238	3.6	9
114	Mechanistic skin penetration model by the COSMOperm method: Routes of permeation, vehicle effects and skin variations in the healthy and compromised skin. *Computational Toxicology*, **2019**, 11, 50-64	3.1	11
113	Ab initio prediction of structuring/mesoscale inhomogeneities in surfactant-free microemulsions and hydrogen-bonding-free microemulsions. *Physical Chemistry Chemical Physics*, **2019**, 21, 8054-8066	3.6	8
112	Prediction of Partition Coefficients of Environmental Toxins Using Computational Chemistry Methods. *ACS Omega*, **2019**, 4, 13772-13781	3.9	15
111	The COSMO and COSMO-RS solvation models. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1338	7.9	108
110	Cocrystal Ternary Phase Diagrams from Density Functional Theory and Solvation Thermodynamics. *Crystal Growth and Design*, **2018**, 18, 5600-5608	3.5	14
109	A refined cavity construction algorithm for the conductor-like screening model. *Journal of Computational Chemistry*, **2018**, 39, 1648-1655	3.5	18
108	COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics. *Computer Aided Chemical Engineering*, **2018**, 43, 9	0.6	2
107	New Molecular Descriptors to Identify Surfactants and Solubilizers from Electron Density Distributions. *Journal of Surfactants and Detergents*, **2018**, 22, 1039	1.9	2
106	High-Throughput Screening of Working Fluids for the Organic Rankine Cycle (ORC) Based on Conductor-like Screening Model for Realistic Solvation (COSMO-RS) and Thermodynamic Process Simulations. *Industrial & Engineering Chemistry Research*, **2017**, 56, 788-798	3.9	19
105	Multi-criteria evaluation of several million working fluids for waste heat recovery by means of Organic Rankine Cycle in passenger cars and heavy-duty trucks. *Applied Energy*, **2017**, 206, 887-899	10.7	35
104	Prediction of cyclohexane-water distribution coefficients with COSMO-RS on the SAMPL5 data set. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 959-967	4.2	40
103	New Developments in Prediction of Solid-State Solubility and Cocrystallization Using COSMO-RS Theory **2016**, 211-233		8

102	COSMO-RS for aqueous solvation and interfaces. *Fluid Phase Equilibria*, **2016**, 407, 152-158	2.5	58
101	Computational Screening of Drug Solvates. *Pharmaceutical Research*, **2016**, 33, 2794-804	4.5	23
100	Quantum chemical insights into the dependence of porphyrin basicity on the meso-aryl substituents: thermodynamics, buckling, reaction sites and molecular flexibility. *Physical Chemistry Chemical Physics*, **2015**, 17, 14096-106	3.6	27
99	Solubility prediction, solvate and cocrystal screening as tools for rational crystal engineering. *Journal of Pharmacy and Pharmacology*, **2015**, 67, 803-11	4.8	68
98	Comment on Phase Behavior of Ternary Mixtures of Water Vanillin Ethanol for Vanillin Extraction via Dissipative Particle Dynamics *Journal of Chemical & Engineering Data*, **2015**, 60, 3437-3438	2.8	1
97	A Comprehensive Comparison of the IEFPCM and SS(V)PE Continuum Solvation Methods with the COSMO Approach. *Journal of Chemical Theory and Computation*, **2015**, 11, 4220-5	6.4	155
96	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
95	Predicting Flash Points of Pure Compounds and Mixtures with COSMO-RS. *Industrial & Engineering Chemistry Research*, **2015**, 54, 12974-12980	3.9	10
94	Calculation of solvation free energies with DCOSMO-RS. *Journal of Physical Chemistry A*, **2015**, 119, 5439-45	2.8	48
93	Prediction of Solubilities and Partition Coefficients in Polymers Using COSMO-RS. *Industrial & Engineering Chemistry Research*, **2014**, 53, 11478-11487	3.9	47
92	Comment on An Improvement to COSMO-SAC for Predicting Thermodynamic Properties *Industrial & Engineering Chemistry Research*, **2014**, 53, 8935-8935	3.9	1
91	First-Principles Prediction of Liquid/Liquid Interfacial Tension. *Journal of Chemical Theory and Computation*, **2014**, 10, 3401-8	6.4	47
90	Consideration of dimerization for property prediction with COSMO-RS-DARE. *Fluid Phase Equilibria*, **2014**, 382, 89-99	2.5	11
89	Prediction of Phospholipid-Water Partition Coefficients of Ionic Organic Chemicals Using the Mechanistic Model COSMOmic. *Journal of Physical Chemistry B*, **2014**, 118, 14833-42	3.4	70
88	Prediction of free energies of hydration with COSMO-RS on the SAMPL4 data set. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 169-73	4.2	18
87	3D-QSAR reloaded: Open3DALIGN meets COSMOsar3D. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
86	Comment on "Computational studies on organic reactivity in ionic liquids" by C. Chiappe and C. S. Pomelli, Phys. Chem. Chem. Phys., 2013, 15, 412. *Physical Chemistry Chemical Physics*, **2013**, 15, 11139-40	3.6	
85	Interpretation of experimental hydrogen-bond enthalpies and entropies from COSMO polarisation charge densities. *Physical Chemistry Chemical Physics*, **2013**, 15, 7147-54	3.6	32

84	COSMOsim3D for drug-similarity, alignment, and molecular field analysis. *Journal of Cheminformatics*, **2012**, 4,	8.6	1
83	Reliable Quantum Chemical Prediction of the Localized/Delocalized Character of Organic Mixed-Valence Radical Anions. From Continuum Solvent Models to Direct-COSMO-RS. *Journal of Chemical Theory and Computation*, **2012**, 8, 4189-203	6.4	70
82	COSMOquick: A Novel Interface for Fast Profile Composition and Its Application to COSMO-RS Solvent Screening Using Multiple Reference Solvents. *Industrial & Engineering Chemistry Research*, **2012**, 51, 14303-14308	3.9	34
81	Comment on Comparison of the a Priori COSMO-RS Models and Group Contribution Methods: Original UNIFAC, Modified UNIFAC(Do), and Modified UNIFAC(Do) Consortium *Industrial & Engineering Chemistry Research*, **2012**, 51, 13538-13540	3.9	4
80	COSMOsar3D: molecular field analysis based on local COSMO profiles. *Journal of Chemical Information and Modeling*, **2012**, 52, 2157-64	6.1	26
79	COSMOsim3D: 3D-similarity and alignment based on COSMO polarization charge densities. *Journal of Chemical Information and Modeling*, **2012**, 52, 2149-56	6.1	14
78	Polarization charge densities provide a predictive quantification of hydrogen bond energies. *Physical Chemistry Chemical Physics*, **2012**, 14, 955-63	3.6	43
77	Rational coformer or solvent selection for pharmaceutical cocrystallization or desolvation. *Journal of Pharmaceutical Sciences*, **2012**, 101, 3687-97	3.9	114
76	Prediction of free energies of hydration with COSMO-RS on the SAMPL3 data set. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 669-73	4.2	11
75	Prediction of the temperature dependence of a polyether water mixture using COSMOtherm. *Fluid Phase Equilibria*, **2011**, 310, 7-10	2.5	16
74	Ionic liquids: predictions of physicochemical properties with experimental and/or DFT-calculated LFER parameters to understand molecular interactions in solution. *Journal of Physical Chemistry B*, **2011**, 115, 6040-50	3.4	49
73	The COSMO and COSMO-RS solvation models. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 699-709	7.9	459
72	Drug Solubility and Reaction Thermodynamics **2010**, 457-476		4
71	Towards a first principles prediction of pK a: COSMO-RS and the cluster-continuum approach. *Molecular Physics*, **2010**, 108, 229-241	1.7	79
70	COSMO-RS: an alternative to simulation for calculating thermodynamic properties of liquid mixtures. *Annual Review of Chemical and Biomolecular Engineering*, **2010**, 1, 101-22	8.9	339
69	Comment on the correct use of continuum solvent models. *Journal of Physical Chemistry A*, **2010**, 114, 13442-4	2.8	326
68	COSMO-RS as a tool for property prediction of IL mixtures A review. *Fluid Phase Equilibria*, **2010**, 294, 31-38	2.5	297
67	Some conclusions regarding the predictions of tautomeric equilibria in solution based on the SAMPL2 challenge. *Journal of Computer-Aided Molecular Design*, **2010**, 24, 621-5	4.2	11

66	Blind prediction test of free energies of hydration with COSMO-RS. *Journal of Computer-Aided Molecular Design*, **2010**, 24, 357-60	4.2	34
65	Predicting the critical micelle concentrations of aqueous solutions of ionic liquids and other ionic surfactants. *Chemistry - A European Journal*, **2009**, 15, 8880-5	4.8	37
64	Prediction of acidity in acetonitrile solution with COSMO-RS. *Journal of Computational Chemistry*, **2009**, 30, 799-810	3.5	140
63	Prediction or partition coefficients and activity coefficients of two branched compounds using COSMOtherm. *Fluid Phase Equilibria*, **2009**, 285, 15-18	2.5	49
62	COSMO-RS as a Predictive Tool for Lipophilicity. *QSAR and Combinatorial Science*, **2009**, 28, 874-877		25
61	Comment on Towards the development of theoretically correct liquid activity coefficient models *Journal of Chemical Thermodynamics*, **2009**, 41, 1312-1313	2.9	2
60	On the performance of continuum solvation methods. A comment on "Universal approaches to solvation modeling". *Accounts of Chemical Research*, **2009**, 42, 489-92; discussion 493-7	24.3	152
59	Prediction of the free energy of hydration of a challenging set of pesticide-like compounds. *Journal of Physical Chemistry B*, **2009**, 113, 4508-10	3.4	66
58	Flüssig vorhergesagt. *Nachrichten Aus Der Chemie*, **2008**, 56, 1034-1036	0.1	
57	Probing carboxylate Gibbs transfer energies via liquid|liquid transfer at triple phase boundary electrodes: ion-transfer voltammetry versus COSMO-RS predictions. *Physical Chemistry Chemical Physics*, **2008**, 10, 3925-33	3.6	32
56	Comment on Refinement of COSMOSAC and the Applications *Industrial & Engineering Chemistry Research*, **2008**, 47, 1351-1352	3.9	2
55	COSMOmic: a mechanistic approach to the calculation of membrane-water partition coefficients and internal distributions within membranes and micelles. *Journal of Physical Chemistry B*, **2008**, 112, 12148-57	3.4	101
54	Butadiene Purification Using Polar Solvents. Analysis of Solution Nonideality Using Data and Estimation Methods. *Industrial & Engineering Chemistry Research*, **2008**, 47, 4996-5004	3.9	16
53	Comments on Performance of COSMO-RS with Sigma Profiles from Different Model Chemistries *Industrial & Engineering Chemistry Research*, **2008**, 47, 987-988	3.9	4
52	Comment on Comparison of Predictivities of Log P Calculation Models Based on Experimental Data for 134 Simple Organic Compounds by Y. Sakuratani, K. Kasai, Y. Noguchi, and J. Yamada, QSAR Comb. Sci. 2007, 26, 109116. *QSAR and Combinatorial Science*, **2008**, 27, 232-233		3
51	Validation of the COSMO-RS electrostatics by Monte-Carlo simulations. *Fluid Phase Equilibria*, **2007**, 261, 162-167	2.5	5
50	Prediction of the vapor pressure and vaporization enthalpy of 1-n-alkyl-3-methylimidazolium-bis-(trifluoromethanesulfonyl) amide ionic liquids. *Physical Chemistry Chemical Physics*, **2007**, 9, 4653-6	3.6	74
49	Solubility of sodium diclofenac in different solvents. *Fluid Phase Equilibria*, **2007**, 261, 140-145	2.5	33

48	Prediction, fine tuning, and temperature extrapolation of a vapor liquid equilibrium using COSMOtherm. *Fluid Phase Equilibria*, **2007**, 260, 183-189	2.5	26
47	Challenge of Drug Solubility Prediction. *Methods and Principles in Medicinal Chemistry*, **2007**, 283-311	0.4	4
46	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions. *Journal of Chemical & Engineering Data*, **2007**, 52, 499-510	2.8	47
45	Prediction of blood-brain partitioning and human serum albumin binding based on COSMO-RS sigma-moments. *Journal of Chemical Information and Modeling*, **2007**, 47, 228-33	6.1	44
44	Accurate prediction of basicity in aqueous solution with COSMO-RS. *Journal of Computational Chemistry*, **2006**, 27, 11-9	3.5	127
43	Comment on "Application of the COSMO-SAC-BP Solvation Model to Predictions of Normal Boiling Temperatures for Environmentally Significant Substances". *Industrial & Engineering Chemistry Research*, **2006**, 45, 3766-3766	3.9	2
42	COSMOsim: bioisosteric similarity based on COSMO-RS sigma profiles. *Journal of Chemical Information and Modeling*, **2006**, 46, 1040-53	6.1	20
41	Calculation of solvent shifts on electronic g-tensors with the conductor-like screening model (COSMO) and its self-consistent generalization to real solvents (direct COSMO-RS). *Journal of Physical Chemistry A*, **2006**, 110, 2235-45	2.8	520
40	Use of surface charges from DFT calculations to predict intestinal absorption. *Journal of Chemical Information and Modeling*, **2005**, 45, 1337-42	6.1	18
39	COSMOfrag: a novel tool for high-throughput ADME property prediction and similarity screening based on quantum chemistry. *Journal of Chemical Information and Modeling*, **2005**, 45, 1169-77	6.1	69
38	Comments on "Performance of a Conductor-Like Screening Model for Real Solvents Model in Comparison to Classical Group Contribution Methods". *Industrial & Engineering Chemistry Research*, **2005**, 44, 7042-7042	3.9	7
37	Vapor–liquid equilibrium prediction at high pressures using activity coefficients at infinite dilution from COSMO-type methods. *Fluid Phase Equilibria*, **2005**, 231, 231-238	2.5	34
36	Molecular Similarity Searching Using COSMO Screening Charges (COSMO/3PP). *Lecture Notes in Computer Science*, **2005**, 175-185	0.9	1
35	Challenges in thermodynamics. *Chemical Engineering and Processing: Process Intensification*, **2004**, 43, 221-238	3.7	34
34	Solvent effects in electronically excited states using the continuum solvation model COSMO in combination with multireference configuration interaction with singles and doubles (MR-CISD). *Theoretical Chemistry Accounts*, **2004**, 111, 78-89	1.9	46
33	Prediction of vapor liquid equilibria using COSMOtherm. *Fluid Phase Equilibria*, **2004**, 217, 53-57	2.5	46
32	Comment on "A critical assessment on two predictive models of binary vapor–liquid equilibrium" by M. Neiman, H. Cheng, V. Parekh, B. Peterson and K. Klier, Phys. Chem. Chem. Phys., 2004, 6, 3474. *Physical Chemistry Chemical Physics*, **2004**, 6, 5081-5081	3.6	4
31	Prediction of halocarbon thermodynamics with COSMO-RS. *Fluid Phase Equilibria*, **2003**, 210, 117-141	2.5	16

30	Prediction of the mutual solubilities of hydrocarbons and water with COSMO-RS. *Fluid Phase Equilibria*, **2003**, 206, 223-235	2.5	89
29	First Principles Calculations of Aqueous pKa Values for Organic and Inorganic Acids Using COSMO-RS Reveal an Inconsistency in the Slope of the pKa Scale. *Journal of Physical Chemistry A*, **2003**, 107, 9380-6	2.8	236
28	Prediction of Infinite Dilution Activity Coefficients of Organic Compounds in Ionic Liquids Using COSMO-RS. *Journal of Chemical & Engineering Data*, **2003**, 48, 475-479	2.8	196
27	Fast solvent screening via quantum chemistry: COSMO-RS approach. *AICHE Journal*, **2002**, 48, 369-385	3.6	1127
26	Use of COSMO-RS for the prediction of adsorption equilibria. *AICHE Journal*, **2002**, 48, 1093-1099	3.6	45
25	COSMOSPACE: Alternative to conventional activity-coefficient models. *AICHE Journal*, **2002**, 48, 2332-2349	3.6	114
24	Prediction of aqueous solubility of drugs and pesticides with COSMO-RS. *Journal of Computational Chemistry*, **2002**, 23, 275-81	3.5	188
23	Prediction of soil sorption coefficients with a conductor-like screening model for real solvents. *Environmental Toxicology and Chemistry*, **2002**, 21, 2562-2566	3.8	29
22	Comments on A Priori Phase Equilibrium Prediction from a Segment Contribution Solvation Model *Industrial & Engineering Chemistry Research*, **2002**, 41, 2330-2331	3.9	14
21	A comparison between the two general sets of linear free energy descriptors of Abraham and Klamt. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 1320-31		102
20	COSMO-RS: a novel view to physiological solvation and partition questions. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 355-65	4.2	100
19	Validation of the COSMO-RS Method: Six Binary Systems. *Industrial & Engineering Chemistry Research*, **2001**, 40, 2371-2378	3.9	34
18	COSMO-RS: a novel and efficient method for the a priori prediction of thermophysical data of liquids. *Fluid Phase Equilibria*, **2000**, 172, 43-72	2.5	855
17	COSMO Implementation in TURBOMOLE: Extension of an efficient quantum chemical code towards liquid systems. *Physical Chemistry Chemical Physics*, **2000**, 2, 2187-2193	3.6	523
16	Insight into Chemical Reactions from First-Principles Simulations: The Mechanism of the Gas-Phase Reaction of OH Radicals with Ketones. *Journal of Physical Chemistry A*, **1998**, 102, 3614-3617	2.8	30
15	Refinement and Parametrization of COSMO-RS. *Journal of Physical Chemistry A*, **1998**, 102, 5074-5085	2.8	1292
14	First principles implementation of solvent effects without outlying charge error. *Journal of Chemical Physics*, **1997**, 106, 6622-6633	3.9	177
13	Treatment of the outlying charge in continuum solvation models. *Journal of Chemical Physics*, **1996**, 105, 9972-9981	3.9	691

12	Estimation of gas-phase hydroxyl radical rate constants of oxygenated compounds based on molecular orbital calculations. *Chemosphere*, **1996**, 32, 717-726	8.4	55
11	Calculation of UV/Vis Spectra in Solution. *The Journal of Physical Chemistry*, **1996**, 100, 3349-3353		208
10	Conductor-like Screening Model for Real Solvents: A New Approach to the Quantitative Calculation of Solvation Phenomena. *The Journal of Physical Chemistry*, **1995**, 99, 2224-2235		2806
9	Zum indirekten Photoabbau chlororganischer Verbindungen durch OH-Radikale in der Atmosphäre. *Environmental Sciences Europe*, **1995**, 7, 275-279		
8	Incorporation of solvent effects into density functional calculations of molecular energies and geometries. *Journal of Chemical Physics*, **1995**, 103, 9312-9320	3.9	682
7	Vorhersage von Gaslöslichkeiten und Verteilungskoeffizienten aufgrund von Molekülorbitalrechnungen (COSMO) unter Berücksichtigung des Lösungsmitteleinflusses. *Chemie-Ingenieur-Technik*, **1995**, 67, 476-479	0.8	17
6	Zum Bioakkumulationspotential von Chlororganika. *Environmental Sciences Europe*, **1993**, 5, 228-234		2
5	On the theory of spin-lattice relaxation due to the hopping motion of light interstitials; the role of excited states. *Journal of Physics Condensed Matter*, **1992**, 4, 3405-3428	1.8	2
4	Tight-binding polarons. II. The interstitial-polaron model. *Journal of Physics Condensed Matter*, **1989**, 1, 3897-3910	1.8	
3	Tight-binding polarons. I. A new variational approach to the molecular-crystal model. *Journal of Physics C: Solid State Physics*, **1988**, 21, 1953-1970		13
2	The Jahn-Teller effect of excited states of hydrogen in metals. *Journal of Physics F: Metal Physics*, **1987**, 17, 47-57		2
1	Quantitative theory of hydrogen diffusion in niobium and tantalum. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1985**, 108, 281-284	2.3	26