Andreas Klamt

List of Publications by Citations

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	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
118	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
117	Refinement and Parametrization of COSMO-RS. *Journal of Physical Chemistry A*, **1998**, 102, 5074-5085	2.8	1292
116	Fast solvent screening via quantum chemistry: COSMO-RS approach. *AICHE Journal*, **2002**, 48, 369-385	3.6	1127
115	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
114	Treatment of the outlying charge in continuum solvation models. *Journal of Chemical Physics*, **1996**, 105, 9972-9981	3.9	691
113	Incorporation of solvent effects into density functional calculations of molecular energies and geometries. *Journal of Chemical Physics*, **1995**, 103, 9312-9320	3.9	682
112	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
111	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
110	The COSMO and COSMO-RS solvation models. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 699-709	7.9	459
109	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
108	Comment on the correct use of continuum solvent models. *Journal of Physical Chemistry A*, **2010**, 114, 13442-4	2.8	326
107	COSMO-RS as a tool for property prediction of IL mixtures—A review. *Fluid Phase Equilibria*, **2010**, 294, 31-38	2.5	297
106	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
105	Calculation of UV/Vis Spectra in Solution. *The Journal of Physical Chemistry*, **1996**, 100, 3349-3353		208
104	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
103	Prediction of aqueous solubility of drugs and pesticides with COSMO-RS. *Journal of Computational Chemistry*, **2002**, 23, 275-81	3.5	188

102	First principles implementation of solvent effects without outlying charge error. *Journal of Chemical Physics*, **1997**, 106, 6622-6633	3.9	177
101	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
100	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
99	Prediction of acidity in acetonitrile solution with COSMO-RS. *Journal of Computational Chemistry*, **2009**, 30, 799-810	3.5	140
98	Accurate prediction of basicity in aqueous solution with COSMO-RS. *Journal of Computational Chemistry*, **2006**, 27, 11-9	3.5	127
97	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
96	Rational coformer or solvent selection for pharmaceutical cocrystallization or desolvation. *Journal of Pharmaceutical Sciences*, **2012**, 101, 3687-97	3.9	114
95	COSMOSPACE: Alternative to conventional activity-coefficient models. *AICHE Journal*, **2002**, 48, 2332-2340	3.9	114
94	The COSMO and COSMO-RS solvation models. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1338	7.9	108
93	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
92	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
91	COSMO-RS: a novel view to physiological solvation and partition questions. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 355-65	4.2	100
90	Prediction of the mutual solubilities of hydrocarbons and water with COSMO-RS. *Fluid Phase Equilibria*, **2003**, 206, 223-235	2.5	89
89	Towards a first principles prediction of pK a: COSMO-RS and the cluster-continuum approach. *Molecular Physics*, **2010**, 108, 229-241	1.7	79
88	3D-QSAR reloaded: Open3DALIGN meets COSMOsar3D. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
87	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
86	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
85	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

84	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
83	Solubility prediction, solvate and cocrystal screening as tools for rational crystal engineering. *Journal of Pharmacy and Pharmacology*, **2015**, 67, 803-11	4.8	68
82	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
81	COSMO-RS for aqueous solvation and interfaces. *Fluid Phase Equilibria*, **2016**, 407, 152-158	2.5	58
80	Estimation of gas-phase hydroxyl radical rate constants of oxygenated compounds based on molecular orbital calculations. *Chemosphere*, **1996**, 32, 717-726	8.4	55
79	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
78	Prediction or partition coefficients and activity coefficients of two branched compounds using COSMOtherm. *Fluid Phase Equilibria*, **2009**, 285, 15-18	2.5	49
77	Calculation of solvation free energies with DCOSMO-RS. *Journal of Physical Chemistry A*, **2015**, 119, 5439-45	2.8	48
76	Prediction of Solubilities and Partition Coefficients in Polymers Using COSMO-RS. *Industrial & Engineering Chemistry Research*, **2014**, 53, 11478-11487	3.9	47
75	First-Principles Prediction of Liquid/Liquid Interfacial Tension. *Journal of Chemical Theory and Computation*, **2014**, 10, 3401-8	6.4	47
74	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
73	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
72	Prediction of vapor liquid equilibria using COSMOtherm. *Fluid Phase Equilibria*, **2004**, 217, 53-57	2.5	46
71	Use of COSMO-RS for the prediction of adsorption equilibria. *AICHE Journal*, **2002**, 48, 1093-1099	3.6	45
70	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
69	Polarization charge densities provide a predictive quantification of hydrogen bond energies. *Physical Chemistry Chemical Physics*, **2012**, 14, 955-63	3.6	43
68	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
67	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

66	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
65	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
64	Blind prediction test of free energies of hydration with COSMO-RS. *Journal of Computer-Aided Molecular Design*, **2010**, 24, 357-60	4.2	34
63	Challenges in thermodynamics. *Chemical Engineering and Processing: Process Intensification*, **2004**, 43, 221-238	3.7	34
62	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
61	Validation of the COSMO-RS Method: Six Binary Systems. *Industrial & Engineering Chemistry Research*, **2001**, 40, 2371-2378	3.9	34
60	Solubility of sodium diclofenac in different solvents. *Fluid Phase Equilibria*, **2007**, 261, 140-145	2.5	33
59	Interpretation of experimental hydrogen-bond enthalpies and entropies from COSMO polarisation charge densities. *Physical Chemistry Chemical Physics*, **2013**, 15, 7147-54	3.6	32
58	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
57	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
56	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
55	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
54	COSMOsar3D: molecular field analysis based on local COSMO profiles. *Journal of Chemical Information and Modeling*, **2012**, 52, 2157-64	6.1	26
53	Prediction, fine tuning, and temperature extrapolation of a vapor liquid equilibrium using COSMOtherm. *Fluid Phase Equilibria*, **2007**, 260, 183-189	2.5	26
52	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
51	COSMO-RS as a Predictive Tool for Lipophilicity. *QSAR and Combinatorial Science*, **2009**, 28, 874-877		25
50	Computational Screening of Drug Solvates. *Pharmaceutical Research*, **2016**, 33, 2794-804	4.5	23
49	COSMOsim: bioisosteric similarity based on COSMO-RS sigma profiles. *Journal of Chemical Information and Modeling*, **2006**, 46, 1040-53	6.1	20

48	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
47	A refined cavity construction algorithm for the conductor-like screening model. *Journal of Computational Chemistry*, **2018**, 39, 1648-1655	3.5	18
46	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
45	Use of surface charges from DFT calculations to predict intestinal absorption. *Journal of Chemical Information and Modeling*, **2005**, 45, 1337-42	6.1	18
44	Vorhersage von Gasl□lichkeiten und Verteilungskoeffizienten aufgrund von Molek□lorbitalrechnungen (COSMO) unter Ber□cksichtigung des L□ungsmitteleinflusses. *Chemie-Ingenieur-Technik*, **1995**, 67, 476-479	0.8	17
43	COSMO-RS based predictions for the SAMPL6 logP challenge. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 385-392	4.2	17
42	Prediction of the temperature dependence of a polyether□water mixture using COSMOtherm. *Fluid Phase Equilibria*, **2011**, 310, 7-10	2.5	16
41	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
40	Prediction of halocarbon thermodynamics with COSMO-RS. *Fluid Phase Equilibria*, **2003**, 210, 117-141	2.5	16
39	Prediction of Partition Coefficients of Environmental Toxins Using Computational Chemistry Methods. *ACS Omega*, **2019**, 4, 13772-13781	3.9	15
38	Cocrystal Ternary Phase Diagrams from Density Functional Theory and Solvation Thermodynamics. *Crystal Growth and Design*, **2018**, 18, 5600-5608	3.5	14
37	COSMOsim3D: 3D-similarity and alignment based on COSMO polarization charge densities. *Journal of Chemical Information and Modeling*, **2012**, 52, 2149-56	6.1	14
36	Comments on □A Priori Phase Equilibrium Prediction from a Segment Contribution Solvation Model□ *Industrial & Engineering Chemistry Research*, **2002**, 41, 2330-2331	3.9	14
35	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
34	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
33	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
32	Consideration of dimerization for property prediction with COSMO-RS-DARE. *Fluid Phase Equilibria*, **2014**, 382, 89-99	2.5	11
31	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

30	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
29	Predicting Flash Points of Pure Compounds and Mixtures with COSMO-RS. *Industrial & Engineering Chemistry Research*, **2015**, 54, 12974-12980	3.9	10
28	COSMOplex: self-consistent simulation of self-organizing inhomogeneous systems based on COSMO-RS. *Physical Chemistry Chemical Physics*, **2019**, 21, 9225-9238	3.6	9
27	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
26	New Developments in Prediction of Solid-State Solubility and Cocrystallization Using COSMO-RS Theory **2016**, 211-233		8
25	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
24	Validation of the COSMO-RS electrostatics by Monte-Carlo simulations. *Fluid Phase Equilibria*, **2007**, 261, 162-167	2.5	5
23	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
22	Drug Solubility and Reaction Thermodynamics **2010**, 457-476		4
21	Comments on Performance of COSMO-RS with Sigma Profiles from Different Model Chemistries *Industrial & Engineering Chemistry Research*, **2008**, 47, 987-988	3.9	4
20	Challenge of Drug Solubility Prediction. *Methods and Principles in Medicinal Chemistry*, **2007**, 283-311	0.4	4
19	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
18	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, 109 116. *QSAR and Combinatorial Science*, **2008**, 27, 232-233		3
17	DRUG SOLUBILITY, REACTION THERMODYNAMICS, AND CO-CRYSTAL SCREENING **2019**, 467-491		2
16	Comment on Towards the development of theoretically correct liquid activity coefficient models *Journal of Chemical Thermodynamics*, **2009**, 41, 1312-1313	2.9	2
15	Comment on Refinement of COSMO SAC and the Applications *Industrial & Engineering Chemistry Research*, **2008**, 47, 1351-1352	3.9	2
14	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
13	Zum Bioakkumulationspotential von Chlororganika. *Environmental Sciences Europe*, **1993**, 5, 228-234		2

12	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
11	The Jahn-Teller effect of excited states of hydrogen in metals. *Journal of Physics F: Metal Physics*, **1987**, 17, 47-57		2
10	COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics. *Computer Aided Chemical Engineering*, **2018**, 43, 9	0.6	2
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8	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
7	Comment on An Improvement to COSMO-SAC for Predicting Thermodynamic Properties *Industrial & Engineering Chemistry Research*, **2014**, 53, 8935-8935	3.9	1
6	COSMOsim3D for drug-similarity, alignment, and molecular field analysis. *Journal of Cheminformatics*, **2012**, 4,	8.6	1
5	Molecular Similarity Searching Using COSMO Screening Charges (COSMO/3PP). *Lecture Notes in Computer Science*, **2005**, 175-185	0.9	1
4	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	
3	Flüssig vorhergesagt. *Nachrichten Aus Der Chemie*, **2008**, 56, 1034-1036	0.1	
2	Zum indirekten Photoabbau chlororganischer Verbindungen durch OH-Radikale in der Atmosphäre. *Environmental Sciences Europe*, **1995**, 7, 275-279		
1	Tight-binding polarons. II. The interstitial-polaron model. *Journal of Physics Condensed Matter*, **1989**, 1, 3897-3910	1.8	