Andreas Klamt

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4942980/publications.pdf

Version: 2024-02-01

112 papers	20,503 citations	41258 49 h-index	22102 113 g-index

124 all docs	124 docs citations	124 times ranked	14889 citing authors

#	Article	IF	Citations
1	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.	2.9	3,325
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Refinement and Parametrization of COSMO-RS. Journal of Physical Chemistry A, 1998, 102, 5074-5085.	1.1	1,577
4	Fast solvent screening via quantum chemistry: COSMO-RS approach. AICHE Journal, 2002, 48, 369-385.	1.8	1,433
5	COSMO-RS: a novel and efficient method for the a priori prediction of thermophysical data of liquids. Fluid Phase Equilibria, 2000, 172, 43-72.	1.4	1,002
6	Incorporation of solvent effects into density functional calculations of molecular energies and geometries. Journal of Chemical Physics, 1995, 103, 9312-9320.	1.2	776
7	Treatment of the outlying charge in continuum solvation models. Journal of Chemical Physics, 1996, 105, 9972-9981.	1.2	771
8	COSMO Implementation in TURBOMOLE: Extension of an efficient quantum chemical code towards liquid systems. Physical Chemistry Chemical Physics, 2000, 2, 2187-2193.	1.3	632
9	Calculation of Solvent Shifts on Electronicg-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, 2235-2245.	1.1	573
10	The COSMO and COSMOâ€RS solvation models. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 699-709.	6.2	571
11	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
12	COSMO-RS: An Alternative to Simulation for Calculating Thermodynamic Properties of Liquid Mixtures. Annual Review of Chemical and Biomolecular Engineering, 2010, 1, 101-122.	3.3	445
13	Comment on the Correct Use of Continuum Solvent Models. Journal of Physical Chemistry A, 2010, 114, 13442-13444.	1.1	432
14	COSMO-RS as a tool for property prediction of IL mixturesâ€"A review. Fluid Phase Equilibria, 2010, 294, 31-38.	1.4	368
15	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, 4220-4225.	2.3	274
16	First Principles Calculations of Aqueous pKaValues for Organic and Inorganic Acids Using COSMOâ˜RS Reveal an Inconsistency in the Slope of the pKaScale. Journal of Physical Chemistry A, 2003, 107, 9380-9386.	1.1	270
17	Calculation of UV/Vis Spectra in Solution. The Journal of Physical Chemistry, 1996, 100, 3349-3353.	2.9	248
18	Prediction of aqueous solubility of drugs and pesticides with COSMO-RS. Journal of Computational Chemistry, 2002, 23, 275-281.	1.5	232

#	Article	IF	Citations
19	Prediction of Infinite Dilution Activity Coefficients of Organic Compounds in Ionic Liquids Using COSMO-RS. Journal of Chemical & Engineering Data, 2003, 48, 475-479.	1.0	215
20	First principles implementation of solvent effects without outlying charge error. Journal of Chemical Physics, 1997, 106, 6622-6633.	1.2	213
21	The <scp>COSMO</scp> and <scp>COSMOâ€RS</scp> solvation models. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1338.	6.2	197
22	On the Performance of Continuum Solvation Methods. A Comment on â€œUniversal Approaches to Solvation Modelingâ€• Accounts of Chemical Research, 2009, 42, 489-492.	7.6	171
23	Prediction of acidity in acetonitrile solution with COSMOâ€RS. Journal of Computational Chemistry, 2009, 30, 799-810.	1.5	168
24	Rational Coformer or Solvent Selection for Pharmaceutical Cocrystallization or Desolvation. Journal of Pharmaceutical Sciences, 2012, 101, 3687-3697.	1.6	150
25	Accurate prediction of basicity in aqueous solution with COSMO-RS. Journal of Computational Chemistry, 2006, 27, 11-19.	1.5	149
26	COSMOSPACE: Alternative to conventional activity-coefficient models. AICHE Journal, 2002, 48, 2332-2349.	1.8	136
27	COSMO-RS: a novel view to physiological solvation and partition questions. Journal of Computer-Aided Molecular Design, 2001, 15, 355-365.	1.3	125
28	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, 1320-1331.	2.8	122
29	COSMOmic: A Mechanistic Approach to the Calculation of Membraneâ^'Water Partition Coefficients and Internal Distributions within Membranes and Micelles. Journal of Physical Chemistry B, 2008, 112, 12148-12157.	1.2	115
30	Prediction of the mutual solubilities of hydrocarbons and water with COSMO-RS. Fluid Phase Equilibria, 2003, 206, 223-235.	1.4	102
31	Solubility prediction, solvate and cocrystal screening as tools for rational crystal engineering. Journal of Pharmacy and Pharmacology, 2015, 67, 803-811.	1.2	102
32	Towards a first principles prediction of pK_a: COSMO-RS and the cluster-continuum approach. Molecular Physics, 2010, 108, 229-241.	0.8	87
33	COSMO-RS for aqueous solvation and interfaces. Fluid Phase Equilibria, 2016, 407, 152-158.	1.4	85
34	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, 4189-4203.	2.3	83
35	Prediction of Phospholipidâ€“Water Partition Coefficients of Ionic Organic Chemicals Using the Mechanistic Model COSMOmic. Journal of Physical Chemistry B, 2014, 118, 14833-14842.	1.2	80
36	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.	1.3	79

#	Article	IF	Citations
37	COSMOfrag:â€‰ A Novel Tool for High-Throughput ADME Property Prediction and Similarity Screening Based on Quantum Chemistry. Journal of Chemical Information and Modeling, 2005, 45, 1169-1177.	2.5	78
38	Prediction of the Free Energy of Hydration of a Challenging Set of Pesticide-Like Compounds. Journal of Physical Chemistry B, 2009, 113, 4508-4510.	1.2	70
39	Estimation of gas-phase hydroxyl radical rate constants of oxygenated compounds based on molecular orbital calculations. Chemosphere, 1996, 32, 717-726.	4.2	65
40	Calculation of Solvation Free Energies with DCOSMO-RS. Journal of Physical Chemistry A, 2015, 119, 5439-5445.	1.1	65
41	Prediction of Solubilities and Partition Coefficients in Polymers Using COSMO-RS. Industrial & Engineering Chemistry Research, 2014, 53, 11478-11487.	1.8	62
42	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, 6040-6050.	1.2	58
43	Prediction of vapor liquid equilibria using COSMOtherm. Fluid Phase Equilibria, 2004, 217, 53-57.	1.4	57
44	First-Principles Prediction of Liquid/Liquid Interfacial Tension. Journal of Chemical Theory and Computation, 2014, 10, 3401-3408.	2.3	56
45	Use of COSMO-RS for the prediction of adsorption equilibria. AICHE Journal, 2002, 48, 1093-1099.	1.8	55
46	Thermochemistry of Chlorobenzenes and Chlorophenols:Â Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions. Journal of Chemical & Engineering Data, 2007, 52, 499-510.	1.0	55
47	Prediction or partition coefficients and activity coefficients of two branched compounds using COSMOtherm. Fluid Phase Equilibria, 2009, 285, 15-18.	1.4	55
48	Prediction of Blood-Î’rain Partitioning and Human Serum Albumin Binding Based on COSMO-RS Ïƒ-Moments. Journal of Chemical Information and Modeling, 2007, 47, 228-233.	2.5	54
49	Polarization charge densities provide a predictive quantification of hydrogen bond energies. Physical Chemistry Chemical Physics, 2012, 14, 955-963.	1.3	54
50	COSMOquick: A Novel Interface for Fast Ïƒ-Profile Composition and Its Application to COSMO-RS Solvent Screening Using Multiple Reference Solvents. Industrial & Engineering Chemistry Research, 2012, 51, 14303-14308.	1.8	50
51	Prediction of cyclohexane-water distribution coefficients with COSMO-RS on the SAMPL5 data set. Journal of Computer-Aided Molecular Design, 2016, 30, 959-967.	1.3	50
52	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.	0.5	46
53	Solubility of sodium diclofenac in different solvents. Fluid Phase Equilibria, 2007, 261, 140-145.	1.4	43
54	Validation of the COSMO-RS Method:Â Six Binary Systems. Industrial & Engineering Chemistry Research, 2001, 40, 2371-2378.	1.8	42

#	Article	IF	Citations
55	Predicting the Critical Micelle Concentrations of Aqueous Solutions of Ionic Liquids and Other Ionic Surfactants. Chemistry - A European Journal, 2009, 15, 8880-8885.	1.7	41
56	A refined cavity construction algorithm for the conductorâ€like screening model. Journal of Computational Chemistry, 2018, 39, 1648-1655.	1.5	41
57	Challenges in thermodynamics. Chemical Engineering and Processing: Process Intensification, 2004, 43, 221-238.	1.8	40
58	Vaporâ€“liquid equilibrium prediction at high pressures using activity coefficients at infinite dilution from COSMO-type methods. Fluid Phase Equilibria, 2005, 231, 231-238.	1.4	40
59	Blind prediction test of free energies of hydration with COSMO-RS. Journal of Computer-Aided Molecular Design, 2010, 24, 357-360.	1.3	39
60	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.	5.1	37
61	COSMOsar3D: Molecular Field Analysis Based on Local COSMO Ïƒ-Profiles. Journal of Chemical Information and Modeling, 2012, 52, 2157-2164.	2.5	36
62	Interpretation of experimental hydrogen-bond enthalpies and entropies from COSMO polarisation charge densities. Physical Chemistry Chemical Physics, 2013, 15, 7147.	1.3	36
63	Insight into Chemical Reactions from First-Principles Simulations:Â The Mechanism of the Gas-Phase Reaction of OH Radicals with Ketones. Journal of Physical Chemistry A, 1998, 102, 3614-3617.	1.1	35
64	Prediction of soil sorption coefficients with a conductorâ€like screening model for real solvents. Environmental Toxicology and Chemistry, 2002, 21, 2562-2566.	2.2	35
65	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.	1.3	34
66	Computational Screening of Drug Solvates. Pharmaceutical Research, 2016, 33, 2794-2804.	1.7	32
67	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, 14096-14106.	1.3	31
68	COSMO-RS based predictions for the SAMPL6 logP challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 385-392.	1.3	30
69	Quantitative theory of hydrogen diffusion in niobium and tantalum. Physics Letters, Section A: General, Atomic and Solid State Physics, 1985, 108, 281-284.	0.9	29
70	Prediction, fine tuning, and temperature extrapolation of a vapor liquid equilibrium using COSMOtherm. Fluid Phase Equilibria, 2007, 260, 183-189.	1.4	28
71	COSMOperm: Mechanistic Prediction of Passive Membrane Permeability for Neutral Compounds and Ions and Its pH Dependence. Journal of Physical Chemistry B, 2020, 124, 3343-3354.	1.2	26
72	COSMO-RS as a Predictive Tool for Lipophilicity. QSAR and Combinatorial Science, 2009, 28, 874-877.	1.5	25

#	Article	IF	Citations
73	Prediction of halocarbon thermodynamics with COSMO-RS. Fluid Phase Equilibria, 2003, 210, 117-141.	1.4	24
74	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.	1.8	24
75	Prediction of Partition Coefficients of Environmental Toxins Using Computational Chemistry Methods. ACS Omega, 2019, 4, 13772-13781.	1.6	24
76	COSMOsim:Â Bioisosteric Similarity Based on COSMO-RS Ïƒ Profiles. Journal of Chemical Information and Modeling, 2006, 46, 1040-1053.	2.5	23
77	Vorhersage von GaslÃ¶slichkeiten und Verteilungskoeffizienten aufgrund von MolekÃ¼lorbitalrechnungen (COSMO) unter BerÃ¼cksichtigung des LÃ¶sungsmitteleinflusses. Chemie-Ingenieur-Technik, 1995, 67, 476-479.	0.4	21
78	COSMOsim3D: 3D-Similarity and Alignment Based on COSMO Polarization Charge Densities. Journal of Chemical Information and Modeling, 2012, 52, 2149-2156.	2.5	21
79	Prediction of free energies of hydration with COSMO-RS on the SAMPL4 data set. Journal of Computer-Aided Molecular Design, 2014, 28, 169-173.	1.3	21
80	Cocrystal Ternary Phase Diagrams from Density Functional Theory and Solvation Thermodynamics. Crystal Growth and Design, 2018, 18, 5600-5608.	1.4	21
81	Use of Surface Charges from DFT Calculations To Predict Intestinal Absorption. Journal of Chemical Information and Modeling, 2005, 45, 1337-1342.	2.5	20
82	Consideration of dimerization for property prediction with COSMO-RS-DARE. Fluid Phase Equilibria, 2014, 382, 89-99.	1.4	20
83	Prediction of the temperature dependence of a polyetherâ€“water mixture using COSMOtherm. Fluid Phase Equilibria, 2011, 310, 7-10.	1.4	19
84	Comments on â€œA Priori Phase Equilibrium Prediction from a Segment Contribution Solvation Modelâ€• Industrial & Engineering Chemistry Research, 2002, 41, 2330-2331.	1.8	17
85	Butadiene Purification Using Polar Solvents. Analysis of Solution Nonideality Using Data and Estimation Methods. Industrial & Engineering Chemistry Research, 2008, 47, 4996-5004.	1.8	17
86	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.	1.8	16
87	Ab initio prediction of structuring/mesoscale inhomogeneities in surfactant-free microemulsions and hydrogen-bonding-free microemulsions. Physical Chemistry Chemical Physics, 2019, 21, 8054-8066.	1.3	16
88	Some conclusions regarding the predictions of tautomeric equilibria in solution based on the SAMPL2 challenge. Journal of Computer-Aided Molecular Design, 2010, 24, 621-625.	1.3	15
89	COSMOplex: self-consistent simulation of self-organizing inhomogeneous systems based on COSMO-RS. Physical Chemistry Chemical Physics, 2019, 21, 9225-9238.	1.3	15
90	Tight-binding polarons. I. A new variational approach to the molecular-crystal model. Journal of Physics C: Solid State Physics, 1988, 21, 1953-1970.	1.5	14

#	Article	IF	Citations
91	Predicting Flash Points of Pure Compounds and Mixtures with COSMO-RS. Industrial & Engineering Chemistry Research, 2015, 54, 12974-12980.	1.8	14
92	Prediction of free energies of hydration with COSMO-RS on the SAMPL3 data set. Journal of Computer-Aided Molecular Design, 2012, 26, 669-673.	1.3	12
93	Comments on â€œPerformance of a Conductor-Like Screening Model for Real Solvents Model in Comparison to Classical Group Contribution Methodsâ€• Industrial & Engineering Chemistry Research, 2005, 44, 7042-7042.	1.8	8
94	Validation of the COSMO-RS electrostatics by Monte-Carlo simulations. Fluid Phase Equilibria, 2007, 261, 162-167.	1.4	6
95	Comment on â€œComparison of the a Priori COSMO-RS Models and Group Contribution Methods: Original UNIFAC, Modified UNIFAC(Do), and Modified UNIFAC(Do) Consortiumâ€• Industrial & Engineering Chemistry Research, 2012, 51, 13538-13540.	1.8	6
96	Comments on â€œPerformance of COSMO-RS with Sigma Profiles from Different Model Chemistriesâ€• Industrial & Engineering Chemistry Research, 2008, 47, 987-988.	1.8	5
97	COSMO-RS: From Quantum Chemistry to Fluid Phase Thermodynamics. Computer Aided Chemical Engineering, 2018, 43, 9.	0.3	5
98	Comment on â€œA critical assessment on two predictive models of binary vaporâ€“liquid equilibriumâ€•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.	1.3	4
99	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.	0.7	3
100	Comment on â€œApplication of the COSMO-SAC-BP Solvation Model to Predictions of Normal Boiling Temperatures for Environmentally Significant Substancesâ€• Industrial & Engineering Chemistry Research, 2006, 45, 3766-3766.	1.8	3
101	Comment on â€œComparison of Predictivities of Logâ€…P Calculation Models Based on Experimental Data for 134 Simple Organic Compoundsâ€•by Y. Sakuratani, K. Kasai, Y. Noguchi, and J. Yamada, QSAR Comb. Sci. 2007, 26, 109â€“116. QSAR and Combinatorial Science, 2008, 27, 232-233.	1.5	3
102	Comment on â€œRefinement of COSMOâ˜SAC and the Applicationsâ€• Industrial & Engineering Chemistry Research, 2008, 47, 1351-1352.	1.8	3
103	COSMOsim3D for drug-similarity, alignment, and molecular field analysis. Journal of Cheminformatics, 2012, 4, .	2.8	3
104	New Molecular Descriptors to Identify Surfactants and Solubilizers from Electron Density Distributions. Journal of Surfactants and Detergents, 2019, 22, 1039-1045.	1.0	3
105	The Jahn-Teller effect of excited states of hydrogen in metals. Journal of Physics F: Metal Physics, 1987, 17, 47-57.	1.6	2
106	Comment on â€œTowards the development of theoretically correct liquid activity coefficient modelsâ€• Journal of Chemical Thermodynamics, 2009, 41, 1312-1313.	1.0	2
107	Comment on â€œAn Improvement to COSMO-SAC for Predicting Thermodynamic Propertiesâ€• Industrial & Engineering Chemistry Research, 2014, 53, 8935-8935.	1.8	2
108	Comment on â€œPhase Behavior of Ternary Mixtures of Waterâ€“Vanillinâ€“Ethanol for Vanillin Extraction via Dissipative Particle Dynamicsâ€• Journal of Chemical & Engineering Data, 2015, 60, 3437-3438.	1.0	1

#	Article	IF	Citations
109	Molecular Similarity Searching Using COSMO Screening Charges (COSMO/3PP). Lecture Notes in Computer Science, 2005, , 175-185.	1.0	1
110	Tight-binding polarons. II. The interstitial-polaron model. Journal of Physics Condensed Matter, 1989, 1, 3897-3910.	0.7	0
111	3D-QSAR reloaded: Open3DALIGN meets COSMOsar3D. Journal of Cheminformatics, 2013, 5, .	2.8	0
112	Comment on â€œComputational studies on organic reactivity in ionic liquidsâ€•by C. Chiappe and C. S. Pomelli, Phys. Chem. Chem. Phys., 2013, 15, 412. Physical Chemistry Chemical Physics, 2013, 15, 11139.	1.3	0