Chieh-Ming Hsieh

List of Publications by Year
in descending order

45	1,166	361413	395702
papers	citations	20 h-index	33 g-index

46	46	46	700
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Prediction of solid solute solubility in supercritical carbon dioxide from PSRK EOS with only input of molecular structure. Journal of Supercritical Fluids, 2022, 180, 105446.	3.2	8
2	Unveiling the mechanism of CO2-driven phase change in amineÂ+ÂwaterÂ+Âglycol ether ternary mixture. Journal of the Taiwan Institute of Chemical Engineers, 2022, 131, 104143.	5.3	2
3	First principles calculations on lithium diffusion near the surface and in the bulk of Fe-doped LiCoPO₄. Physical Chemistry Chemical Physics, 2022, 24, 1147-1155.	2.8	5
4	Measurement and modeling of metoclopramide hydrochloride (anti-emetic drug) solubility in supercritical carbon dioxide. Arabian Journal of Chemistry, 2022, 15, 103876.	4.9	23
5	Phase equilibrium modeling of mixtures containing conformationally flexible molecules with the COSMO-SAC model. Journal of Molecular Liquids, 2022, 356, 118896.	4.9	4
6	Modeling of phase separation solvent for CO2 capture using COSMO-SAC model. Journal of the Taiwan Institute of Chemical Engineers, 2022, 135, 104362.	5.3	3
7	Particle Size and Crystal Habit Modification of Active Pharmaceutical Ingredient Using Cooling Sonocrystallization: A Case Study of Probenecid. Crystal Research and Technology, 2021, 56, 2000182.	1.3	3
8	Computational study on the effect of steric hindrance in functionalised Zr-based metal-organic frameworks on hydrocarbon storage and separation. Molecular Simulation, 2021, 47, 565-574.	2.0	5
9	Hydrogenated Anatase and Rutile TiO₂ for Sodium-Ion Battery Anodes. ACS Applied Energy Materials, 2021, 4, 5738-5746.	5.1	22
10	Investigating lithium intercalation and diffusion in Nb-doped TiO2 by first principles calculations. Journal of the Taiwan Institute of Chemical Engineers, 2021, 125, 314-322.	5.3	11
11	Towards design of phase separation solvent for CO2 capture using COSMO-SAC model. Journal of Molecular Liquids, 2021, 336, 116229.	4.9	6
12	Measurement and modeling of solubility of gliclazide (hypoglycemic drug) and captopril (antihypertension drug) in supercritical carbon dioxide. Journal of Supercritical Fluids, 2021, 174, 105244.	3.2	32
13	Preparation of Microcellular Foams by Supercritical Carbon Dioxide: A Case Study of Thermoplastic Polyurethane 70A. Processes, 2021, 9, 1650.	2.8	2
14	Measurement and Correlation of Solubility of Methylsalicylic Acid Isomers in Supercritical Carbon Dioxide. Journal of Chemical & Engineering Data, 2021, 66, 280-289.	1.9	6
15	Prediction of solid solute solubility in supercritical carbon dioxide with and without organic cosolvents from PSRK EOS. Journal of Supercritical Fluids, 2020, 158, 104735.	3.2	11
16	First-principles prediction of solid solute solubility in supercritical carbon dioxide using PR+COSMOSAC EOS. Fluid Phase Equilibria, 2020, 522, 112755.	2.5	17
17	A Benchmark Open-Source Implementation of COSMO-SAC. Journal of Chemical Theory and Computation, 2020, 16, 2635-2646.	5.3	74
18	Improvement to PR+COSMOSAC EOS for Predicting the Vapor Pressure of Nonelectrolyte Organic Solids and Liquids. Industrial & Engineering Chemistry Research, 2019, 58, 5030-5040.	3.7	20

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19	SkaSim â€“ Scalable HPC Software for Molecular Simulation in the Chemical Industry. Chemie-Ingenieur-Technik, 2018, 90, 295-306.	0.8	7
20	Prediction of solid-liquid-gas equilibrium for binary mixtures of carbon dioxide + organic compounds from approaches based on the COSMO-SAC model. Journal of Supercritical Fluids, 2018, 133, 318-329.	3.2	9
21	Prediction of Gas and Liquid Solubility in Organic Polymers Based on the PR+COSMOSAC Equation of State. Industrial & Engineering Chemistry Research, 2018, 57, 10628-10639.	3.7	6
22	First-Principles Study of Lithium Intercalation and Diffusion in Oxygen-Defective Titanium Dioxide. Journal of Physical Chemistry C, 2018, 122, 19447-19454.	3.1	30
23	Understanding the Differing Fluid Phase Behavior of Cyclohexane + Benzene and Their Hydroxylated or Aminated Forms. Journal of Physical Chemistry B, 2017, 121, 5374-5384.	2.6	5
24	Comprehensive Assessment of COSMO-SAC Models for Predictions of Fluid-Phase Equilibria. Industrial & Engineering Chemistry Research, 2017, 56, 9868-9884.	3.7	56
25	Prediction of solid solute solubility in supercritical carbon dioxide with organic cosolvents from the PR+COSMOSAC equation of state. Fluid Phase Equilibria, 2017, 431, 48-57.	2.5	23
26	A Critical Evaluation on the Performance of COSMO-SAC Models for Vaporâ€“Liquid and Liquidâ€“Liquid Equilibrium Predictions Based on Different Quantum Chemical Calculations. Industrial & Engineering Chemistry Research, 2016, 55, 9312-9322.	3.7	53
27	Vaporâ€“liquid equilibrium measurements of the binary mixtures CO2+acetone and CO2+pentanones. Journal of Supercritical Fluids, 2015, 100, 160-166.	3.2	23
28	Improved Prediction of Vapor Pressure for Pure Liquids and Solids from the PR+COSMOSAC Equation of State. Industrial & Engineering Chemistry Research, 2015, 54, 10115-10125.	3.7	18
29	Considering the dispersive interactions in the COSMO-SAC model for more accurate predictions of fluid phase behavior. Fluid Phase Equilibria, 2014, 367, 109-116.	2.5	54
30	Vaporâ€“Liquid Equilibria of CO₂ + C1â€“C5 Alcohols from the Experiment and the COSMO-SAC Model. Journal of Chemical & Engineering Data, 2013, 58, 3420-3429.	1.9	20
31	Fluidâ€phase coexistence for the oxidation of <scp>CO</scp>₂ expanded cyclohexane: Experiment, molecular simulation, and <scp>COSMO</scp>â€<scp>SAC</scp>. AICHE Journal, 2013, 59, 2236-2250.	3.6	9
32	Rapid determination of entropy and free energy of mixtures from molecular dynamics simulations with the two-phase thermodynamic model. Physical Chemistry Chemical Physics, 2012, 14, 15206.	2.8	35
33	Firstâ€principles prediction of phase equilibria using the PR + COSMOSAC equation of state. Asia-Pacific Journal of Chemical Engineering, 2012, 7, S1.	1.5	11
34	A Predictive Model for the Solubility and Octanolâ^'Water Partition Coefficient of Pharmaceuticals. Journal of Chemical & Engineering Data, 2011, 56, 936-945.	1.9	44
35	First-Principles Prediction of Vaporâ^'Liquidâ^'Liquid Equilibrium from the PR+COSMOSAC Equation of State. Industrial & Engineering Chemistry Research, 2011, 50, 1496-1503.	3.7	15
36	Prediction of miscibility gaps in water/ether mixtures using COSMO-SAC model. Fluid Phase Equilibria, 2011, 310, 19-24.	2.5	26

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37	Prediction of liquidâ€“liquid equilibrium from the Pengâ€“Robinson+COSMOSAC equation of state. Chemical Engineering Science, 2010, 65, 1955-1963.	3.8	34
38	Improvements of COSMO-SAC for vaporâ€“liquid and liquidâ€“liquid equilibrium predictions. Fluid Phase Equilibria, 2010, 297, 90-97.	2.5	249
39	Towards the development of theoretically correct liquid activity coefficient models. Journal of Chemical Thermodynamics, 2009, 41, 1145-1153.	2.0	17
40	Reply to â€œComment on â€œTowards the development of theoretically correct liquid activity coefficient modelsâ€â€. Journal of Chemical Thermodynamics, 2009, 41, 1314-1316.	2.0	1
41	Prediction of 1-octanolâ€“water partition coefficient and infinite dilution activity coefficient in water from the PR+COSMOSAC model. Fluid Phase Equilibria, 2009, 285, 8-14.	2.5	27
42	First-Principles Predictions of Vaporâˆ’Liquid Equilibria for Pure and Mixture Fluids from the Combined Use of Cubic Equations of State and Solvation Calculations. Industrial & Engineering Chemistry Research, 2009, 48, 3197-3205.	3.7	46
43	Determination of cubic equation of state parameters for pure fluids from first principle solvation calculations. AICHE Journal, 2008, 54, 2174-2181.	3.6	39
44	Solvation and chemical engineering thermodynamics. Journal of the Taiwan Institute of Chemical Engineers, 2007, 38, 467-476.	1.4	27
45	Efficient and accurate solvation energy calculation from polarizable continuum models. Journal of Chemical Physics, 2006, 125, 124103.	3.0	23