

Chieh-Ming Hsieh

List of Publications by Year in descending order

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45
papers

1,166
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361045

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times ranked

700
citing authors

#	ARTICLE	IF	CITATIONS
1	Prediction of solid solute solubility in supercritical carbon dioxide from PSRK EOS with only input of molecular structure. <i>Journal of Supercritical Fluids</i> , 2022, 180, 105446.	1.6	8
2	Unveiling the mechanism of CO ₂ -driven phase change in amine+water+glycol ether ternary mixture. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2022, 131, 104143.	2.7	2
3	First principles calculations on lithium diffusion near the surface and in the bulk of Fe-doped LiCoPO ₄ . <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1147-1155.	1.3	5
4	Measurement and modeling of metoclopramide hydrochloride (anti-emetic drug) solubility in supercritical carbon dioxide. <i>Arabian Journal of Chemistry</i> , 2022, 15, 103876.	2.3	23
5	Phase equilibrium modeling of mixtures containing conformationally flexible molecules with the COSMO-SAC model. <i>Journal of Molecular Liquids</i> , 2022, 356, 118896.	2.3	4
6	Modeling of phase separation solvent for CO ₂ capture using COSMO-SAC model. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2022, 135, 104362.	2.7	3
7	Particle Size and Crystal Habit Modification of Active Pharmaceutical Ingredient Using Cooling Sonocrystallization: A Case Study of Probenecid. <i>Crystal Research and Technology</i> , 2021, 56, 2000182.	0.6	3
8	Computational study on the effect of steric hindrance in functionalised Zr-based metal-organic frameworks on hydrocarbon storage and separation. <i>Molecular Simulation</i> , 2021, 47, 565-574.	0.9	5
9	Hydrogenated Anatase and Rutile TiO ₂ for Sodium-Ion Battery Anodes. <i>ACS Applied Energy Materials</i> , 2021, 4, 5738-5746.	2.5	22
10	Investigating lithium intercalation and diffusion in Nb-doped TiO ₂ by first principles calculations. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2021, 125, 314-322.	2.7	11
11	Towards design of phase separation solvent for CO ₂ capture using COSMO-SAC model. <i>Journal of Molecular Liquids</i> , 2021, 336, 116229.	2.3	6
12	Measurement and modeling of solubility of gliclazide (hypoglycemic drug) and captopril (antihypertension drug) in supercritical carbon dioxide. <i>Journal of Supercritical Fluids</i> , 2021, 174, 105244.	1.6	32
13	Preparation of Microcellular Foams by Supercritical Carbon Dioxide: A Case Study of Thermoplastic Polyurethane 70A. <i>Processes</i> , 2021, 9, 1650.	1.3	2
14	Measurement and Correlation of Solubility of Methylsalicylic Acid Isomers in Supercritical Carbon Dioxide. <i>Journal of Chemical & Engineering Data</i> , 2021, 66, 280-289.	1.0	6
15	Prediction of solid solute solubility in supercritical carbon dioxide with and without organic cosolvents from PSRK EOS. <i>Journal of Supercritical Fluids</i> , 2020, 158, 104735.	1.6	11
16	First-principles prediction of solid solute solubility in supercritical carbon dioxide using PR+COSMOSAC EOS. <i>Fluid Phase Equilibria</i> , 2020, 522, 112755.	1.4	17
17	A Benchmark Open-Source Implementation of COSMO-SAC. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2635-2646.	2.3	74
18	Improvement to PR+COSMOSAC EOS for Predicting the Vapor Pressure of Nonelectrolyte Organic Solids and Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 5030-5040.	1.8	20

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19	SkaSim – Scalable HPC Software for Molecular Simulation in the Chemical Industry. <i>Chemie-Ingenieur-Technik</i> , 2018, 90, 295-306.	0.4	7
20	Prediction of solid-liquid-gas equilibrium for binary mixtures of carbon dioxide + organic compounds from approaches based on the COSMO-SAC model. <i>Journal of Supercritical Fluids</i> , 2018, 133, 318-329.	1.6	9
21	Prediction of Gas and Liquid Solubility in Organic Polymers Based on the PR+COSMOSAC Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 10628-10639.	1.8	6
22	First-Principles Study of Lithium Intercalation and Diffusion in Oxygen-Defective Titanium Dioxide. <i>Journal of Physical Chemistry C</i> , 2018, 122, 19447-19454.	1.5	30
23	Understanding the Differing Fluid Phase Behavior of Cyclohexane + Benzene and Their Hydroxylated or Aminated Forms. <i>Journal of Physical Chemistry B</i> , 2017, 121, 5374-5384.	1.2	5
24	Comprehensive Assessment of COSMO-SAC Models for Predictions of Fluid-Phase Equilibria. <i>Industrial & Engineering Chemistry Research</i> , 2017, 56, 9868-9884.	1.8	56
25	Prediction of solid solute solubility in supercritical carbon dioxide with organic cosolvents from the PR+COSMOSAC equation of state. <i>Fluid Phase Equilibria</i> , 2017, 431, 48-57.	1.4	23
26	A Critical Evaluation on the Performance of COSMO-SAC Models for Vapor–Liquid and Liquid–Liquid Equilibrium Predictions Based on Different Quantum Chemical Calculations. <i>Industrial & Engineering Chemistry Research</i> , 2016, 55, 9312-9322.	1.8	53
27	Vapor–liquid equilibrium measurements of the binary mixtures CO ₂ +acetone and CO ₂ +pentanones. <i>Journal of Supercritical Fluids</i> , 2015, 100, 160-166.	1.6	23
28	Improved Prediction of Vapor Pressure for Pure Liquids and Solids from the PR+COSMOSAC Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2015, 54, 10115-10125.	1.8	18
29	Considering the dispersive interactions in the COSMO-SAC model for more accurate predictions of fluid phase behavior. <i>Fluid Phase Equilibria</i> , 2014, 367, 109-116.	1.4	54
30	Vapor–Liquid Equilibria of CO ₂ + C ₁ –C ₅ Alcohols from the Experiment and the COSMO-SAC Model. <i>Journal of Chemical & Engineering Data</i> , 2013, 58, 3420-3429.	1.0	20
31	Fluid–phase coexistence for the oxidation of CO ₂ expanded cyclohexane: Experiment, molecular simulation, and COSMO-SAC. <i>AIChE Journal</i> , 2013, 59, 2236-2250.	1.8	9
32	Rapid determination of entropy and free energy of mixtures from molecular dynamics simulations with the two-phase thermodynamic model. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15206.	1.3	35
33	First-principles prediction of phase equilibria using the PR + COSMOSAC equation of state. <i>Asia-Pacific Journal of Chemical Engineering</i> , 2012, 7, S1.	0.8	11
34	A Predictive Model for the Solubility and Octanol–Water Partition Coefficient of Pharmaceuticals. <i>Journal of Chemical & Engineering Data</i> , 2011, 56, 936-945.	1.0	44
35	First-Principles Prediction of Vapor–Liquid–Liquid Equilibrium from the PR+COSMOSAC Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2011, 50, 1496-1503.	1.8	15
36	Prediction of miscibility gaps in water/ether mixtures using COSMO-SAC model. <i>Fluid Phase Equilibria</i> , 2011, 310, 19-24.	1.4	26

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37	Prediction of liquid-liquid equilibrium from the Peng-Robinson+COSMOSAC equation of state. Chemical Engineering Science, 2010, 65, 1955-1963.	1.9	34
38	Improvements of COSMO-SAC for vapor-liquid and liquid-liquid equilibrium predictions. Fluid Phase Equilibria, 2010, 297, 90-97.	1.4	249
39	Towards the development of theoretically correct liquid activity coefficient models. Journal of Chemical Thermodynamics, 2009, 41, 1145-1153.	1.0	17
40	Reply to "Comment on "Towards the development of theoretically correct liquid activity coefficient models". Journal of Chemical Thermodynamics, 2009, 41, 1314-1316.	1.0	1
41	Prediction of 1-octanol-water partition coefficient and infinite dilution activity coefficient in water from the PR+COSMOSAC model. Fluid Phase Equilibria, 2009, 285, 8-14.	1.4	27
42	First-Principles Predictions of Vapor-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.	1.8	46
43	Determination of cubic equation of state parameters for pure fluids from first principle solvation calculations. AIChE Journal, 2008, 54, 2174-2181.	1.8	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.	1.2	23