Chieh-Ming Hsieh

List of Publications by Year
in descending order

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45 papers	1,166 citations	361045 20 h-index	395343 33 g-index
46 all docs	46 docs citations	46 times ranked	700 citing authors

#	Article	IF	Citations
1	Improvements of COSMO-SAC for vaporâ€“liquid and liquidâ€“liquid equilibrium predictions. Fluid Phase Equilibria, 2010, 297, 90-97.	1.4	249
2	A Benchmark Open-Source Implementation of COSMO-SAC. Journal of Chemical Theory and Computation, 2020, 16, 2635-2646.	2.3	74
3	Comprehensive Assessment of COSMO-SAC Models for Predictions of Fluid-Phase Equilibria. Industrial & Engineering Chemistry Research, 2017, 56, 9868-9884.	1.8	56
4	Considering the dispersive interactions in the COSMO-SAC model for more accurate predictions of fluid phase behavior. Fluid Phase Equilibria, 2014, 367, 109-116.	1.4	54
5	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.	1.8	53
6	First-Principles Predictions of Vaporâ^'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
7	A Predictive Model for the Solubility and Octanolâ^'Water Partition Coefficient of Pharmaceuticals. Journal of Chemical & Engineering Data, 2011, 56, 936-945.	1.0	44
8	Determination of cubic equation of state parameters for pure fluids from first principle solvation calculations. AICHE Journal, 2008, 54, 2174-2181.	1.8	39
9	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.	1.3	35
10	Prediction of liquidâ€“liquid equilibrium from the Pengâ€“Robinson+COSMOSAC equation of state. Chemical Engineering Science, 2010, 65, 1955-1963.	1.9	34
11	Measurement and modeling of solubility of gliclazide (hypoglycemic drug) and captopril (antihypertension drug) in supercritical carbon dioxide. Journal of Supercritical Fluids, 2021, 174, 105244.	1.6	32
12	First-Principles Study of Lithium Intercalation and Diffusion in Oxygen-Defective Titanium Dioxide. Journal of Physical Chemistry C, 2018, 122, 19447-19454.	1.5	30
13	Solvation and chemical engineering thermodynamics. Journal of the Taiwan Institute of Chemical Engineers, 2007, 38, 467-476.	1.4	27
14	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.	1.4	27
15	Prediction of miscibility gaps in water/ether mixtures using COSMO-SAC model. Fluid Phase Equilibria, 2011, 310, 19-24.	1.4	26
16	Efficient and accurate solvation energy calculation from polarizable continuum models. Journal of Chemical Physics, 2006, 125, 124103.	1.2	23
17	Vaporâ€“liquid equilibrium measurements of the binary mixtures CO2+acetone and CO2+pentanones. Journal of Supercritical Fluids, 2015, 100, 160-166.	1.6	23
18	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.	1.4	23

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19	Measurement and modeling of metoclopramide hydrochloride (anti-emetic drug) solubility in supercritical carbon dioxide. Arabian Journal of Chemistry, 2022, 15, 103876.	2.3	23
20	Hydrogenated Anatase and Rutile TiO₂ for Sodium-Ion Battery Anodes. ACS Applied Energy Materials, 2021, 4, 5738-5746.	2.5	22
21	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.	1.0	20
22	Improvement to PR+COSMOSAC EOS for Predicting the Vapor Pressure of Nonelectrolyte Organic Solids and Liquids. Industrial & Engineering Chemistry Research, 2019, 58, 5030-5040.	1.8	20
23	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.	1.8	18
24	Towards the development of theoretically correct liquid activity coefficient models. Journal of Chemical Thermodynamics, 2009, 41, 1145-1153.	1.0	17
25	First-principles prediction of solid solute solubility in supercritical carbon dioxide using PR+COSMOSAC EOS. Fluid Phase Equilibria, 2020, 522, 112755.	1.4	17
26	First-Principles Prediction of Vaporâ^'Liquidâ^'Liquid Equilibrium from the PR+COSMOSAC Equation of State. Industrial & Engineering Chemistry Research, 2011, 50, 1496-1503.	1.8	15
27	Firstâ€principles prediction of phase equilibria using the PR + COSMOSAC equation of state. Asia-Pacific Journal of Chemical Engineering, 2012, 7, S1.	0.8	11
28	Prediction of solid solute solubility in supercritical carbon dioxide with and without organic cosolvents from PSRK EOS. Journal of Supercritical Fluids, 2020, 158, 104735.	1.6	11
29	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.	2.7	11
30	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.	1.8	9
31	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.	1.6	9
32	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.	1.6	8
33	SkaSim â€“ Scalable HPC Software for Molecular Simulation in the Chemical Industry. Chemie-Ingenieur-Technik, 2018, 90, 295-306.	0.4	7
34	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.	1.8	6
35	Towards design of phase separation solvent for CO2 capture using COSMO-SAC model. Journal of Molecular Liquids, 2021, 336, 116229.	2.3	6
36	Measurement and Correlation of Solubility of Methylsalicylic Acid Isomers in Supercritical Carbon Dioxide. Journal of Chemical & Engineering Data, 2021, 66, 280-289.	1.0	6

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37	Understanding the Differing Fluid Phase Behavior of Cyclohexane + Benzene and Their Hydroxylated or Aminated Forms. Journal of Physical Chemistry B, 2017, 121, 5374-5384.	1.2	5
38	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.	0.9	5
39	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.	1.3	5
40	Phase equilibrium modeling of mixtures containing conformationally flexible molecules with the COSMO-SAC model. Journal of Molecular Liquids, 2022, 356, 118896.	2.3	4
41	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.	0.6	3
42	Modeling of phase separation solvent for CO2 capture using COSMO-SAC model. Journal of the Taiwan Institute of Chemical Engineers, 2022, 135, 104362.	2.7	3
43	Preparation of Microcellular Foams by Supercritical Carbon Dioxide: A Case Study of Thermoplastic Polyurethane 70A. Processes, 2021, 9, 1650.	1.3	2
44	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.	2.7	2
45	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.	1.0	1