Simon MÃ¼ller

List of Publications by Year
in descending order

11	229	1039880 9	1199470 12
papers	citations	h-index	g-index

12	12	12	224
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Thermodynamic and Transport Properties Modeling of Deep Eutectic Solvents: A Review on g^E-Models, Equations of State, and Molecular Dynamics. Journal of Chemical & Engineering Data, 2020, 65, 943-967.	1.0	52
2	Influence of Inorganic Salts on the Phase Equilibrium of Triton X-114 Aqueous Two-Phase Systems. Journal of Chemical & Engineering Data, 2016, 61, 1496-1501.	1.0	38
3	Development of a COSMOâ€RS based model for the calculation of phase equilibria in electrolyte systems. AICHE Journal, 2018, 64, 272-285.	1.8	36
4	Physicochemical Characterization and Simulation of the Solidâ€“Liquid Equilibrium Phase Diagram of Terpene-Based Eutectic Solvent Systems. Molecules, 2021, 26, 1801.	1.7	18
5	Flexible heuristic algorithm for automatic molecule fragmentation: application to the UNIFAC group contribution model. Journal of Cheminformatics, 2019, 11, 57.	2.8	17
6	Calculation of thermodynamic equilibria with the predictive electrolyte model COSMO-RS-ES: Improvements for low permittivity systems. Fluid Phase Equilibria, 2020, 506, 112368.	1.4	17
7	Prediction of Solvation Free Energies of Ionic Solutes in Neutral Solvents. Journal of Physical Chemistry A, 2020, 124, 4171-4181.	1.1	15
8	Evaluation and refinement of the novel predictive electrolyte model COSMO-RS-ES based on solid-liquid equilibria of salts and Gibbs free energies of transfer of ions. Fluid Phase Equilibria, 2019, 483, 165-174.	1.4	14
9	An open source COSMO-RS implementation and parameterization supporting the efficient implementation of multiple segment descriptors. Fluid Phase Equilibria, 2022, 560, 113472.	1.4	12
10	On the analogy between the restricted primitive model and capacitor circuits: Semi-empirical alternatives for over- and underscreening in the calculation of mean ionic activity coefficients. Journal of Molecular Liquids, 2021, 326, 115204.	2.3	5
11	On the analogy between the restricted primitive model and capacitor circuits. Part II: A generalized Gibbs-Duhem consistent extension of the Pitzer-Debye-HÃ¼ckel term with corrections for low and variable relative permittivity. Journal of Molecular Liquids, 2022, 360, 119398.	2.3	4