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	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
2	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
3	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
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	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
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	Flexible heuristic algorithm for automatic molecule fragmentation: application to the UNIFAC group contribution model. Journal of Cheminformatics, 2019, 11, 57.	2.8	17
9	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
10	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
11	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