

Yunhao Sun

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	A computational study of water in $\text{LiO} \cdot \text{Zr} \cdot \text{MOFs}$: Diffusion, hydrogen bonding network, and confinement effect. <i>AIChE Journal</i> , 2021, 67, e17035.	3.6	16
2	Modeling Interfacial Properties with Spot-DGT-ePC-SAFT for Binary Mixtures Including Ionic Liquid-Based Systems. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 4484-4497.	3.7	5
3	Modeling interfacial properties of ionic liquids with ePC-SAFT combined with density gradient theory. <i>Fluid Phase Equilibria</i> , 2021, 536, 112984.	2.5	5
4	Accelerate the ePC-SAFT-DFT Calculation with the Chebyshev Pseudospectral Collocation Method. <i>Industrial & Engineering Chemistry Research</i> , 2021, 60, 9269-9285.	3.7	7
5	Simultaneous representation of thermodynamic properties and viscosities of ILs/DESs+co-solvent systems by Eyring-NRTL model. <i>Fluid Phase Equilibria</i> , 2021, 547, 113176.	2.5	4
6	Accelerate the Electrolyte Perturbed-Chain Statistical Associating Fluid Theory's Density Functional Theory Calculation With the Chebyshev Pseudo-Spectral Collocation Method. Part II. Spherical Geometry and Anderson Mixing. <i>Frontiers in Chemistry</i> , 2021, 9, 801551.	3.6	4
7	CO ₂ separation using a hybrid choline-2-pyrrolidine-carboxylic acid/polyethylene glycol/water absorbent. <i>Applied Energy</i> , 2020, 257, 113962.	10.1	17
8	How to detect possible pitfalls in ePC-SAFT modelling: Extension to ionic liquids. <i>Fluid Phase Equilibria</i> , 2020, 519, 112641.	2.5	12
9	Screening Deep Eutectic Solvents for CO ₂ Capture With COSMO-RS. <i>Frontiers in Chemistry</i> , 2020, 8, 82.	3.6	36
10	How to Detect Possible Pitfalls in ePC-SAFT Modeling. 2. Extension to Binary Mixtures of 96 Ionic Liquids with CO ₂ , H ₂ S, CO, O ₂ , CH ₄ , N ₂ , and H ₂ . <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 21579-21591.	3.7	12
11	Modeling Thermodynamic Derivative Properties and Gas Solubility of Ionic Liquids with ePC-SAFT. <i>Industrial & Engineering Chemistry Research</i> , 2019, 58, 8401-8417.	3.7	33
12	Unique Structures and Vibrational Spectra of Protic Ionic Liquids Confined in TiO ₂ Slits: The Role of Interfacial Hydrogen Bonds. <i>Langmuir</i> , 2018, 34, 13449-13458.	3.5	9
13	Modeling Viscosity of Ionic Liquids with Electrolyte Perturbed-Chain Statistical Associating Fluid Theory and Free Volume Theory. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 8784-8801.	3.7	28
14	Wetting control through topography and surface hydrophilic/hydrophobic property changes by coarse grained simulation. <i>Molecular Simulation</i> , 2017, 43, 1202-1208.	2.0	5
15	Screening ionic liquids for developing advanced immobilization technology for CO ₂ separation. <i>Frontiers in Chemistry</i> , 0, 10, .	3.6	1