Zeynep Pinar Haslak

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Assessing CH4/N2 separation potential of MOFs, COFs, IL/MOF, MOF/Polymer, and COF/Polymer composites. Chemical Engineering Journal, 2022, 428, 131239.	12.7	89
2	Accelerating discovery of COFs for CO2 capture and H2 purification using structurally guided computational screening. Chemical Engineering Journal, 2022, 427, 131574.	12.7	26
3	Multi-scale computational screening to accelerate discovery of IL/COF composites for CO2/N2 separation. Separation and Purification Technology, 2022, 287, 120578.	7.9	12
4	Composites of porous materials with ionic liquids: Synthesis, characterization, applications, and beyond. Microporous and Mesoporous Materials, 2022, 332, 111703.	4.4	30
5	Exploring covalent organic frameworks for H2S+CO2 separation from natural gas using efficient computational approaches. Journal of CO2 Utilization, 2022, 62, 102077.	6.8	4
6	An Integrated Computational–Experimental Hierarchical Approach for the Rational Design of an IL/UiOâ€66 Composite Offering Infinite CO ₂ Selectivity. Advanced Functional Materials, 2022, 32, .	14.9	16
7	Doubling CO2/N2 separation performance of CuBTC by incorporation of 1-n-ethyl-3-methylimidazolium diethyl phosphate. Microporous and Mesoporous Materials, 2021, 316, 110947.	4.4	19
8	SAMPL7 blind challenge: quantum–mechanical prediction of partition coefficients and acid dissociation constants for small drug-like molecules. Journal of Computer-Aided Molecular Design, 2021, 35, 841-851.	2.9	10
9	Using Atomic Charges to Describe the p <i>K</i> _a of Carboxylic Acids. Journal of Chemical Information and Modeling, 2021, 61, 2733-2743.	5.4	18
10	Combined GCMC, MD, and DFT Approach for Unlocking the Performances of COFs for Methane Purification. Industrial & Engineering Chemistry Research, 2021, 60, 12999-13012.	3.7	14
11	Elucidation of the atroposelectivity in the synthesis of axially chiral thiohydantoin derivatives. Organic and Biomolecular Chemistry, 2020, 18, 2233-2241.	2.8	6
12	A DFT approach to discriminate the antagonist and partial agonist activity of ligands binding to the NMDA receptor. Molecular Physics, 2018, 116, 323-337.	1.7	1