

Allison L Dzubak

List of Publications by Year in descending order

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Version: 2024-02-01

12
papers

2,531
citations

840776

11
h-index

1058476

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docs citations

14
times ranked

3997
citing authors

#	ARTICLE	IF	CITATIONS
1	MnNiO ₃ revisited with modern theoretical and experimental methods. <i>Journal of Chemical Physics</i> , 2017, 147, 174703.	3.0	10
2	Cooperative insertion of CO ₂ in diamine-appended metal-organic frameworks. <i>Nature</i> , 2015, 519, 303-308.	27.8	1,026
3	CO ₂ induced phase transitions in diamine-appended metal-organic frameworks. <i>Chemical Science</i> , 2015, 6, 5177-5185.	7.4	45
4	Oxidation of ethane to ethanol by N ₂ O in a metal-organic framework with coordinatively unsaturated iron(II) sites. <i>Nature Chemistry</i> , 2014, 6, 590-595.	13.6	398
5	Design of a Metal-Organic Framework with Enhanced Back Bonding for Separation of N ₂ and CH ₄ . <i>Journal of the American Chemical Society</i> , 2014, 136, 698-704.	13.7	157
6	Uranyl-Peroxide Nanocapsules in Aqueous Solution: Force Field Development and First Applications. <i>Journal of Physical Chemistry C</i> , 2014, 118, 24730-24740.	3.1	22
7	CO ₂ Adsorption in Fe ₂ (dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 12230-12240.	3.1	45
8	Reversible CO Binding Enables Tunable CO/H ₂ and CO/N ₂ Separations in Metal-Organic Frameworks with Exposed Divalent Metal Cations. <i>Journal of the American Chemical Society</i> , 2014, 136, 10752-10761.	13.7	210
9	The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2013, 135, 7402-7405.	13.7	208
10	Ab initio carbon capture in open-site metal-organic frameworks. <i>Nature Chemistry</i> , 2012, 4, 810-816.	13.6	310
11	A Combined Spectroscopic and Computational Study of a High-Spin $S = 7/2$ Diiron Complex with a Short Iron-Iron Bond. <i>Inorganic Chemistry</i> , 2012, 51, 728-736.	4.0	45
12	Assessing Metal-Metal Multiple Bonds in Cr ₂ Cr, Mo ₂ Mo, and W ₂ W Compounds and a Hypothetical U ₂ U Compound: A Quantum Chemical Study Comparing DFT and Multireference Methods. <i>Chemistry - A European Journal</i> , 2012, 18, 1737-1749.	3.3	53