

# Allison L Dzubak

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/2378707/publications.pdf>

Version: 2024-02-01

12  
papers

2,531  
citations

840776

11  
h-index

1058476

14  
g-index

14  
all docs

14  
docs citations

14  
times ranked

3997  
citing authors

#	ARTICLE	IF	CITATIONS
1	Cooperative insertion of CO <sub>2</sub> in diamine-appended metal-organic frameworks. <i>Nature</i> , 2015, 519, 303-308.	27.8	1,026
2	Oxidation of ethane to ethanol by N <sub>2</sub> O in a metal-organic framework with coordinatively unsaturated iron(II) sites. <i>Nature Chemistry</i> , 2014, 6, 590-595.	13.6	398
3	Ab initio carbon capture in open-site metal-organic frameworks. <i>Nature Chemistry</i> , 2012, 4, 810-816.	13.6	310
4	Reversible CO Binding Enables Tunable CO/H <sub>2</sub> and CO/N <sub>2</sub> 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
5	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
6	Design of a Metal-Organic Framework with Enhanced Back Bonding for Separation of N <sub>2</sub> and CH <sub>4</sub> . <i>Journal of the American Chemical Society</i> , 2014, 136, 698-704.	13.7	157
7	Assessing Metal-Metal Multiple Bonds in Cr <sub>2</sub> , Cr, Mo <sub>2</sub> , Mo, and W <sub>2</sub> , W Compounds and a Hypothetical U <sub>2</sub> Compound: A Quantum Chemical Study Comparing DFT and Multireference Methods. <i>Chemistry - A European Journal</i> , 2012, 18, 1737-1749.	3.3	53
8	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
9	CO <sub>2</sub> Adsorption in Fe <sub>2</sub> (dobdc): A Classical Force Field Parameterized from Quantum Mechanical Calculations. <i>Journal of Physical Chemistry C</i> , 2014, 118, 12230-12240.	3.1	45
10	CO <sub>2</sub> induced phase transitions in diamine-appended metal-organic frameworks. <i>Chemical Science</i> , 2015, 6, 5177-5185.	7.4	45
11	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
12	MnNiO <sub>3</sub> revisited with modern theoretical and experimental methods. <i>Journal of Chemical Physics</i> , 2017, 147, 174703.	3.0	10