

Haoyu S Yu

List of Publications by Year in descending order

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Version: 2024-02-01

17
papers

2,056
citations

623188

14
h-index

794141

19
g-index

20
all docs

20
docs citations

20
times ranked

2422
citing authors

#	ARTICLE	IF	CITATIONS
1	General Theory of Fragment Linking in Molecular Design: Why Fragment Linking Rarely Succeeds and How to Improve Outcomes. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 450-462.	2.3	21
2	Advancing Free-Energy Calculations of Metalloenzymes in Drug Discovery via Implementation of LFMM Potentials. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6926-6937.	2.3	8
3	Heats of Adsorption of N ₂ , CO, Ar, and CH ₄ versus Coverage on the Zr-Based MOF NU-1000: Measurements and DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2019, 123, 6586-6591.	1.5	8
4	Rigorous Free Energy Perturbation Approach to Estimating Relative Binding Affinities between Ligands with Multiple Protonation and Tautomeric States. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 424-435.	2.3	36
5	Äœber Oxidationszahlœbergrenzen in der Chemie. <i>Angewandte Chemie</i> , 2018, 130, 3297-3300.	1.6	15
6	On the Upper Limits of Oxidation States in Chemistry. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 3242-3245.	7.2	46
7	Energetics of van der Waals Adsorption on the MetalœOrganic Framework NU-1000 with Zr ₆ -oxo, Hydroxo, and Aqua Nodes. <i>Journal of the American Chemical Society</i> , 2018, 140, 328-338.	6.6	11
8	Revised M06-L functional for improved accuracy on chemical reaction barrier heights, noncovalent interactions, and solid-state physics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 8487-8492.	3.3	167
9	Oxidation State 10 Exists. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9004-9006.	7.2	42
10	Oxidation State 10 Exists. <i>Angewandte Chemie</i> , 2016, 128, 9150-9152.	1.6	21
11	Perspective: Kohn-Sham density functional theory descending a staircase. <i>Journal of Chemical Physics</i> , 2016, 145, 130901.	1.2	243
12	MN15: A KohnœSham global-hybrid exchangeœcorrelation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. <i>Chemical Science</i> , 2016, 7, 5032-5051.	3.7	858
13	MN15-L: A New Local Exchange-Correlation Functional for KohnœSham Density Functional Theory with Broad Accuracy for Atoms, Molecules, and Solids. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1280-1293.	2.3	364
14	Components of the Bond Energy in Polar Diatomic Molecules, Radicals, and Ions Formed by Group-1 and Group-2 Metal Atoms. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2968-2983.	2.3	30
15	Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals. <i>ACS Catalysis</i> , 2015, 5, 2070-2080.	5.5	28
16	Nonseparable exchangeœcorrelation functional for molecules, including homogeneous catalysis involving transition metals. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 12146-12160.	1.3	111
17	What Dominates the Error in the CaO Diatomic Bond Energy Predicted by Various Approximate ExchangeœCorrelation Functionals?. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2291-2305.	2.3	17