Haoyu S Yu

List of Publications by Year
in descending order

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17	2,056	623188	794141
papers	citations	14 h-index	19 g-index

20	20	20	2422
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	MN15: A Kohnâ€“Sham global-hybrid exchangeâ€“correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions. Chemical Science, 2016, 7, 5032-5051.	3.7	858
2	MN15-L: A New Local Exchange-Correlation Functional for Kohnâ€“Sham Density Functional Theory with Broad Accuracy for Atoms, Molecules, and Solids. Journal of Chemical Theory and Computation, 2016, 12, 1280-1293.	2.3	364
3	Perspective: Kohn-Sham density functional theory descending a staircase. Journal of Chemical Physics, 2016, 145, 130901.	1.2	243
4	Revised M06-L functional for improved accuracy on chemical reaction barrier heights, noncovalent interactions, and solid-state physics. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 8487-8492.	3.3	167
5	Nonseparable exchangeâ€“correlation functional for molecules, including homogeneous catalysis involving transition metals. Physical Chemistry Chemical Physics, 2015, 17, 12146-12160.	1.3	111
6	On the Upper Limits of Oxidation States in Chemistry. Angewandte Chemie - International Edition, 2018, 57, 3242-3245.	7.2	46
7	Oxidation State 10 Exists. Angewandte Chemie - International Edition, 2016, 55, 9004-9006.	7.2	42
8	Rigorous Free Energy Perturbation Approach to Estimating Relative Binding Affinities between Ligands with Multiple Protonation and Tautomeric States. Journal of Chemical Theory and Computation, 2019, 15, 424-435.	2.3	36
9	Components of the Bond Energy in Polar Diatomic Molecules, Radicals, and Ions Formed by Group-1 and Group-2 Metal Atoms. Journal of Chemical Theory and Computation, 2015, 11, 2968-2983.	2.3	30
10	Density Functional Theory of the Water Splitting Reaction on Fe(0): Comparison of Local and Nonlocal Correlation Functionals. ACS Catalysis, 2015, 5, 2070-2080.	5.5	28
11	Oxidation State 10 Exists. Angewandte Chemie, 2016, 128, 9150-9152.	1.6	21
12	General Theory of Fragment Linking in Molecular Design: Why Fragment Linking Rarely Succeeds and How to Improve Outcomes. Journal of Chemical Theory and Computation, 2021, 17, 450-462.	2.3	21
13	What Dominates the Error in the CaO Diatomic Bond Energy Predicted by Various Approximate Exchangeâ€“Correlation Functionals?. Journal of Chemical Theory and Computation, 2014, 10, 2291-2305.	2.3	17
14	Ãœber Oxidationszahlâ€Obergrenzen in der Chemie. Angewandte Chemie, 2018, 130, 3297-3300.	1.6	15
15	Energetics of van der Waals Adsorption on the Metalâ€“Organic Framework NU-1000 with Zr₆-oxo, Hydroxo, and Aqua Nodes. Journal of the American Chemical Society, 2018, 140, 328-338.	6.6	11
16	Heats of Adsorption of N₂, CO, Ar, and CH₄ versus Coverage on the Zr-Based MOF NU-1000: Measurements and DFT Calculations. Journal of Physical Chemistry C, 2019, 123, 6586-6591.	1.5	8
17	Advancing Free-Energy Calculations of Metalloenzymes in Drug Discovery via Implementation of LFMM Potentials. Journal of Chemical Theory and Computation, 2020, 16, 6926-6937.	2.3	8