Adam H Steeves

List of Publications by Year
in descending order

19	458	687363 13	794594 19
papers	citations	h-index	g-index

20	20	20	351
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. Chemical Reviews, 2021, 121, 9927-10000.	47.7	110
2	Leveraging Cheminformatics Strategies for Inorganic Discovery: Application to Redox Potential Design. Industrial & Engineering Chemistry Research, 2017, 56, 4898-4910.	3.7	45
3	Harder, better, faster, stronger: Large-scale QM and QM/MM for predictive modeling in enzymes and proteins. Current Opinion in Structural Biology, 2022, 72, 9-17.	5.7	42
4	Revealing quantum mechanical effects in enzyme catalysis with large-scale electronic structure simulation. Reaction Chemistry and Engineering, 2019, 4, 298-315.	3.7	33
5	The Proteinâ€™s Role in Substrate Positioning and Reactivity for Biosynthetic Enzyme Complexes: The Case of SyrB2/SyrB1. ACS Catalysis, 2019, 9, 4930-4943.	11.2	28
6	Darlingâ€“Dennison resonance and Coriolis coupling in the bending overtones of the Ã¬Au1 state of acetylene, C2H2. Journal of Chemical Physics, 2008, 129, 054304.	3.0	25
7	Harnessing Organic Ligand Libraries for First-Principles Inorganic Discovery: Indium Phosphide Quantum Dot Precursor Design Strategies. Chemistry of Materials, 2017, 29, 3632-3643.	6.7	24
8	Stretch-bend combination polyads in the Ã1Au state of acetylene, C2H2. Journal of Molecular Spectroscopy, 2009, 256, 256-278.	1.2	23
9	Cis-trans isomerization in the S1 state of acetylene: Identification of cis-well vibrational levels. Journal of Chemical Physics, 2011, 134, 244310.	3.0	21
10	Quantum Mechanical Description of Electrostatics Provides a Unified Picture of Catalytic Action Across Methyltransferases. Journal of Physical Chemistry Letters, 2019, 10, 3779-3787.	4.6	21
11	Electronic Signatures of Large Amplitude Motions:Â Dipole Moments of Vibrationally Excited Local-Bend and Local-Stretch States of S0Acetyleneâ€. Journal of Physical Chemistry B, 2006, 110, 18912-18920.	2.6	20
12	The Ã¹A_u state of acetylene: ungerade vibrational levels in the region 45,800â€“46,550â€‰cm^{â^'1}. Molecular Physics, 2012, 110, 2707-2723.	1.7	19
13	Direct observation of the symmetric stretching modes ofÃ¹A_uacetylene by pulsed supersonic jet laser induced fluorescence. Molecular Physics, 2008, 106, 1867-1877.	1.7	17
14	Millimeter-wave-detected, millimeter-wave optical polarization spectroscopy. Journal of Chemical Physics, 2005, 123, 141102.	3.0	8
15	Influence of the Greater Protein Environment on the Electrostatic Potential in Metalloenzyme Active Sites: The Case of Formate Dehydrogenase. Journal of Physical Chemistry B, 2022, 126, 4069-4079.	2.6	8
16	Large-Scale Screening Reveals That Geometric Structure Matters More Than Electronic Structure in the Bioinspired Catalyst Design of Formate Dehydrogenase Mimics. ACS Catalysis, 2022, 12, 383-396.	11.2	5
17	Communication: Observation of local-bender eigenstates in acetylene. Journal of Chemical Physics, 2015, 143, 071101.	3.0	3
18	Simplified Cartesian Basis Model for Intrapolyad Emission Intensities in the Bent-to-Linear Electronic Transition of Acetylene. Journal of Physical Chemistry A, 2015, 119, 857-865.	2.5	3

#	Article	IF	Citations
19	Quantifying the Longâ€Range Coupling of Electronic Properties in Proteins with ab initio Molecular Dynamics**. Chemistry Methods, 2021, 1, 362-373.	3.8	3