

Prachi Sharma

List of Publications by Year in descending order

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Version: 2024-02-01

11
papers

917
citations

933447

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1281871

11
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12
all docs

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docs citations

12
times ranked

1241
citing authors

#	ARTICLE	IF	CITATIONS
1	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5925-5964.	5.3	661
2	Density matrix renormalization group pair-density functional theory (DMRG-PDFT): singlet–triplet gaps in polyacenes and polyacetylenes. <i>Chemical Science</i> , 2019, 10, 1716-1723.	7.4	69
3	Bimetallic nickel-lutetium complexes: tuning the properties and catalytic hydrogenation activity of the Ni site by varying the Lu coordination environment. <i>Chemical Science</i> , 2019, 10, 3375-3384.	7.4	44
4	Valence $\pi\pi^*$ Excitations in Benzene Studied by Multiconfiguration Pair-Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 75-81.	4.6	29
5	Magnetic Coupling in a Tris-hydroxo-Bridged Chromium Dimer Occurs through Ligand Mediated Superexchange in Conjunction with Through-Space Coupling. <i>Journal of the American Chemical Society</i> , 2020, 142, 16644-16650.	13.7	26
6	Active Space Dependence in Multiconfiguration Pair-Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 660-669.	5.3	20
7	Multiconfiguration pair-density functional theory investigation of the electronic spectrum of MnO_4^- . <i>Journal of Chemical Physics</i> , 2018, 148, 124305.	3.0	18
8	Multiple Bonds in Uranium–Transition Metal Complexes. <i>Inorganic Chemistry</i> , 2019, 58, 10139-10147.	4.0	16
9	Determination of the SmO ⁺ bond energy by threshold photodissociation of the cryogenically cooled ion. <i>Journal of Chemical Physics</i> , 2021, 155, 174303.	3.0	15
10	Metal–Metal Bonding in Actinide Dimers: U_2 and U_2^{+} . <i>Journal of the American Chemical Society</i> , 2021, 143, 17023-17028.	13.7	11
11	Activation of Low-Valent, Multiply M–M Bonded Group VI Dimers toward Catalytic Olefin Metathesis via Surface Organometallic Chemistry. <i>Organometallics</i> , 2020, 39, 1035-1045.	2.3	8