Prajay Patel

List of Publications by Year
in descending order

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		1478280	1281743
14	121	6	11
papers	citations	h-index	g-index

22	22	22	148
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tale of Three Molecular Nitrides: Mononuclear Vanadium (V) and (IV) Nitrides As Well As a Mixed-Valence Trivanadium Nitride Having a V₃N₄ Double-Diamond Core. Journal of the American Chemical Society, 2022, 144, 10201-10219.	6.6	3
2	Integrated Experimental and Computational K-Edge X-ray Absorption Near-Edge Structure Analysis of Vanadium Catalysts. Journal of Physical Chemistry C, 2022, 126, 11949-11962.	1.5	7
3	Computational Investigation of the Role of Active Site Heterogeneity for a Supported Organovanadium(III) Hydrogenation Catalyst. ACS Catalysis, 2021, 11, 7257-7269.	5.5	16
4	Single-Molecule Kinetics of Styrene Hydrogenation on Silica-Supported Vanadium: The Role of Disorder for Single-Atom Catalysts. Journal of Physical Chemistry C, 2021, 125, 20286-20300.	1.5	10
5	Ab initio composite methodologies: Their significance for the chemistry community. Annual Reports in Computational Chemistry, 2021, 17, 113-161.	0.9	4
6	Prediction of p K a s of Late Transitionâ€Metal Hydrides via a QM/QM Approach. Journal of Computational Chemistry, 2020, 41, 171-183.	1.5	4
7	Domainâ€based local pair natural orbital methods within the correlation consistent composite approach. Journal of Computational Chemistry, 2020, 41, 800-813.	1.5	14
8	Electrochemical Investigation of Low-Valent Multiply Mâ‰¡M Bonded Group VI Dimers: A Standard Chemical Reduction Leads to an Unexpected Product. Organometallics, 2020, 39, 4430-4436.	1.1	6
9	Computational chemistry considerations in catalysis: Regioselectivity and metal-ligand dissociation. Catalysis Today, 2020, 358, 422-429.	2.2	5
10	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 495-510.	1.3	11
11	Charge Stabilization in High-Potential Zinc Porphyrin-Fullerene via Axial Ligation of Tetrathiafulvalene. Journal of Physical Chemistry C, 2018, 122, 13636-13647.	1.5	16
12	SAMPL6 hostâ€“guest challenge: binding free energies via a multistep approach. Journal of Computer-Aided Molecular Design, 2018, 32, 1097-1115.	1.3	16
13	Lithium-Ion Battery Materials as Tunable, â€œRedox Non-Innocentâ€•Catalyst Supports. ACS Catalysis, 0, , 7233-7242.	5.5	6
14	Computational Aspects of Single-Molecule Kinetics for Coupled Catalytic Cycles: A Spectral Analysis. Journal of Physical Chemistry A, 0, , .	1.1	2