Tom Ichibha

List of Publications by Year
in descending order

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Version: 2024-02-01

20 papers	380 citations	1040056 9 h-index	794594 19 g-index
20 all docs	20 docs citations	20 times ranked	580 citing authors

#	Article	IF	Citations
1	A Stable, Narrow-Gap Oxyfluoride Photocatalyst for Visible-Light Hydrogen Evolution and Carbon Dioxide Reduction. Journal of the American Chemical Society, 2018, 140, 6648-6655.	13.7	139
2	Undoped Layered Perovskite Oxynitride Li₂LaTa₂O₆N for Photocatalytic CO₂ Reduction with Visible Light. Angewandte Chemie - International Edition, 2018, 57, 8154-8158.	13.8	66
3	Twoâ€Dimensional Perovskite Oxynitride K₂LaTa₂O₆N with an H⁺/K⁺ Exchangeability in Aqueous Solution Forming a Stable Photocatalyst for Visibleâ€Light H₂ Evolution. Angewandte Chemie - International Edition, 2020, 59, 9736-9743.	13.8	33
4	Light Absorption Properties and Electronic Band Structures of Lead Titanium Oxyfluoride Photocatalysts Pb₂Ti₄O₉F₂ and Pb₂Ti₂O_{5.4}F_{1.2}. Journal of Physical Chemistry C, 2018, 122, 26506-26511.	3.1	31
5	Undoped Layered Perovskite Oxynitride Li₂LaTa₂O₆N for Photocatalytic CO₂ Reduction with Visible Light. Angewandte Chemie, 2018, 130, 8286-8290.	2.0	17
6	New Insight into the Ground State of FePc: A Diffusion Monte Carlo Study. Scientific Reports, 2017, 7, 2011.	3.3	15
7	Adhesion of electrodes on diamond (111) surface: A DFT study. Diamond and Related Materials, 2018, 81, 168-175.	3.9	14
8	Ab Initio Evaluation of Complexation Energies for Cyclodextrin-Drug Inclusion Complexes. ACS Omega, 2020, 5, 19371-19376.	3.5	12
9	Ab Initio Search of Polymer Crystals with High Thermal Conductivity. Chemistry of Materials, 2019, 31, 4649-4656.	6.7	9
10	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml revisited with a many-body ab initio theoretical approach. Physical Review Materials, 2021, 5, .	2.4	9
11	Ti interstitial flows giving rutile TiO2 reoxidation process enhancement in (001) surface. Physical Review Materials, 2019, 3, .	2.4	7
12	Inconsistencies in ab initio evaluations of non-additive contributions of DNA stacking energies. Chemical Physics, 2020, 529, 110554.	1.9	6
13	Diffusion Monte Carlo Study on Relative Stabilities of Boron Nitride Polymorphs. Journal of Physical Chemistry C, 2022, 126, 6000-6007.	3.1	6
14	Candidate structure for the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">H</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> -PRE phase of solid hydrogen. Physical Review B, 2021, 104, .	3.2	5
15	Twoâ€Dimensional Perovskite Oxynitride K₂LaTa₂O₆N with an H⁺/K⁺ Exchangeability in Aqueous Solution Forming a Stable Photocatalyst for Visibleâ€Light H₂ Evolution. Angewandte Chemie, 2020, 132, 9823-9830.	2.0	4
16	A new ab initio modeling scheme for the ion self-diffusion coefficient applied to the Îµ-Cu₃Sn phase of the Cuâ€“Sn alloy. Physical Chemistry Chemical Physics, 2019, 21, 5158-5164.	2.8	2
17	GaN bandgap bias caused by semi-core treatment in pseudopotentials analyzed by the diffusion Monte Carlo method. AIP Advances, 2021, 11, 025225.	1.3	2
18	A quantum annealing approach to ionic diffusion in solids. Scientific Reports, 2021, 11, 7261.	3.3	2

#	Article	IF	Citations
19	Making the most of data: Quantum Monte Carlo postanalysis revisited. Physical Review E, 2022, 105, 045313.	2.1	1
20	Diffusion Monte Carlo evaluation of disiloxane linearisation barrier. Physical Chemistry Chemical Physics, 2022, , .	2.8	0