

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	Diffusion Monte Carlo evaluation of disiloxane linearisation barrier. Physical Chemistry Chemical Physics, 2022, , .	2.8	0
2	Diffusion Monte Carlo Study on Relative Stabilities of Boron Nitride Polymorphs. Journal of Physical Chemistry C, 2022, 126, 6000-6007.	3.1	6
3	Making the most of data: Quantum Monte Carlo postanalysis revisited. Physical Review E, 2022, 105, 045313.	2.1	1
4	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
5	A quantum annealing approach to ionic diffusion in solids. Scientific Reports, 2021, 11, 7261.	3.3	2
6	$\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{Cr} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 3 \langle \text{mml:mn} \rangle 2 \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle$ revisited with a many-body $\langle i \rangle$ ab initio $\langle /i \rangle$ theoretical approach. Physical Review Materials, 2021, 5, .	2.4	4
7	Candidate structure for the $\langle \text{mml:math} \text{ xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \text{ mathvariant="normal"} \rangle \text{H} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle$ -PRE phase of solid hydrogen. Physical Review B, 2021, 104, .	3.2	5
8	Inconsistencies in ab initio evaluations of non-additive contributions of DNA stacking energies. Chemical Physics, 2020, 529, 110554.	1.9	6
9	$\langle i \rangle$ Ab Initio $\langle /i \rangle$ Evaluation of Complexation Energies for Cyclodextrin-Drug Inclusion Complexes. ACS Omega, 2020, 5, 19371-19376.	3.5	12
10	Two-dimensional Perovskite Oxynitride $\text{K}_{2}\text{LaTa}_{2}\text{O}_{6}\text{N}$ with an $\text{H}^{\text{sup}}/\text{K}^{\text{sup}}$ Exchangeability in Aqueous Solution Forming a Stable Photocatalyst for Visible-Light H_{2} Evolution. Angewandte Chemie, 2020, 132, 9823-9830.	2.0	4
11	Two-dimensional Perovskite Oxynitride $\text{K}_{2}\text{LaTa}_{2}\text{O}_{6}\text{N}$ with an $\text{H}^{\text{sup}}/\text{K}^{\text{sup}}$ Exchangeability in Aqueous Solution Forming a Stable Photocatalyst for Visible-Light H_{2} Evolution. Angewandte Chemie - International Edition, 2020, 59, 9736-9743.	13.8	33
12	Ab Initio Search of Polymer Crystals with High Thermal Conductivity. Chemistry of Materials, 2019, 31, 4649-4656.	6.7	9
13	A new $\langle i \rangle$ ab initio $\langle /i \rangle$ modeling scheme for the ion self-diffusion coefficient applied to the $\mu\text{-Cu}_{3}\text{Sn}$ phase of the Cu-Sn alloy. Physical Chemistry Chemical Physics, 2019, 21, 5158-5164.	2.8	2
14	Ti interstitial flows giving rutile TiO_{2} reoxidation process enhancement in (001) surface. Physical Review Materials, 2019, 3, .	2.4	7
15	Adhesion of electrodes on diamond (111) surface: A DFT study. Diamond and Related Materials, 2018, 81, 168-175.	3.9	14
16	Light Absorption Properties and Electronic Band Structures of Lead Titanium Oxyfluoride Photocatalysts $\text{Pb}_{2}\text{Ti}_{4}\text{O}_{9}\text{F}_{2}$ and $\text{Pb}_{2}\text{Ti}_{2}\text{O}_{5.4}\text{F}_{1.2}$. Journal of Physical Chemistry C, 2018, 122, 26506-26511.	3.1	31
17	Undoped Layered Perovskite Oxynitride $\text{Li}_{2}\text{LaTa}_{2}\text{O}_{6}\text{N}$ for Photocatalytic CO_{2} Reduction with Visible Light. Angewandte Chemie, 2018, 130, 8286-8290.	2.0	17
18	Undoped Layered Perovskite Oxynitride $\text{Li}_{2}\text{LaTa}_{2}\text{O}_{6}\text{N}$ for Photocatalytic CO_{2} Reduction with Visible Light. Angewandte Chemie - International Edition, 2018, 57, 8154-8158.	13.8	66

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19	A Stable, Narrow-Gap Oxyfluoride Photocatalyst for Visible-Light Hydrogen Evolution and Carbon Dioxide Reduction. <i>Journal of the American Chemical Society</i> , 2018, 140, 6648-6655.	13.7	139
20	New Insight into the Ground State of FePc: A Diffusion Monte Carlo Study. <i>Scientific Reports</i> , 2017, 7, 2011.	3.3	15