Xuecheng Shao

List of Publications by Year
in descending order

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22 papers	450 citations	687220 13 h-index	713332 21 g-index
22 all docs	22 docs citations	22 times ranked	502 citing authors

#	Article	IF	Citations
1	Direct-gap semiconducting tri-layer silicene with 29% photovoltaic efficiency. Nano Energy, 2018, 51, 489-495.	8.2	46
2	Efficient potential-tuning strategy through p-type doping for designing cathodes with ultrahigh energy density. National Science Review, 2020, 7, 1768-1775.	4.6	43
3	ATLAS: A real-space finite-difference implementation of orbital-free density functional theory. Computer Physics Communications, 2016, 200, 87-95.	3.0	42
4	Polyethylene Glycolâ€“Na⁺ Interface of Vanadium Hexacyanoferrate Cathode for Highly Stable Rechargeable Aqueous Sodium-Ion Battery. ACS Applied Materials & Interfaces, 2019, 11, 28762-28768.	4.0	41
5	A symmetry-orientated divide-and-conquer method for crystal structure prediction. Journal of Chemical Physics, 2022, 156, 014105.	1.2	40
6	<scp>DFTpy</scp>: An efficient and objectâ€oriented platform for orbitalâ€free <scp>DFT</scp> simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, .	6.2	34
7	High-Pressure Evolution of Unexpected Chemical Bonding and Promising Superconducting Properties of YB₆. Journal of Physical Chemistry C, 2018, 122, 27820-27828.	1.5	23
8	Large-scale ab initio simulations for periodic system. Computer Physics Communications, 2018, 233, 78-83.	3.0	23
9	Electronic Topological Transition in Ag2Te at High-pressure. Scientific Reports, 2015, 5, 14681.	1.6	20
10	Pressure-stabilized divalent ozonide CaO3 and its impact on Earthâ€™s oxygen cycles. Nature Communications, 2020, 11, 4702.	5.8	20
11	Structure evolution of chromium-doped boron clusters: toward the formation of endohedral boron cages. RSC Advances, 2019, 9, 2870-2876.	1.7	18
12	Revised Huang-Carter nonlocal kinetic energy functional for semiconductors and their surfaces. Physical Review B, 2021, 104, .	1.1	15
13	Efficient DFT Solver for Nanoscale Simulations and Beyond. Journal of Physical Chemistry Letters, 2021, 12, 4134-4139.	2.1	13
14	eQE 2.0: Subsystem DFT beyond GGA functionals. Computer Physics Communications, 2021, 269, 108122.	3.0	13
15	An automated predictor for identifying transition states in solids. Npj Computational Materials, 2020, 6, .	3.5	12
16	Ab initio electronic structure calculations using a real-space Chebyshev-filtered subspace iteration method. Journal of Physics Condensed Matter, 2019, 31, 455901.	0.7	11
17	First-principles study of high-pressure phase stability and superconductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mathvariant="normal">I</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2019, 100, .	1.1	9
18	GGA-Level Subsystem DFT Achieves Sub-kcal/mol Accuracy Intermolecular Interactions by Mimicking Nonlocal Functionals. Journal of Chemical Theory and Computation, 2021, 17, 3455-3461.	2.3	9

#	Article	IF	Citations
19	Nonlocal and nonadiabatic Pauli potential for time-dependent orbital-free density functional theory. Physical Review B, 2021, 104, .	1.1	8
20	O (N log N) scaling method to evaluate the ionâ€“electron potential of crystalline solids. Journal of Chemical Physics, 2016, 145, 184110.	1.2	7
21	Many-body van der Waals interactions in wet MoS₂ surfaces. Electronic Structure, 2022, 4, 024001.	1.0	2
22	Stability and mechanical properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">W</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow><mml:mi mathvariant="normal">Mo</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mrow><mml:mn>4.2</mml:mn></mml:mrow></mml:msub></mml:math>		