Hongyan Wang

List of Publications by Year
in descending order

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38	833	516710 16	501196 28
papers	citations	h-index	g-index

38	38	38	1024
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Novel two-dimensional semiconductor SnP₃: high stability, tunable bandgaps and high carrier mobility explored using first-principles calculations. Journal of Materials Chemistry A, 2018, 6, 11890-11897.	10.3	146
2	Two-dimensional Blue-AsP monolayers with tunable direct band gap and ultrahigh carrier mobility show promising high-performance photovoltaic properties. Nanoscale, 2019, 11, 8260-8269.	5.6	70
3	Flexible, auxetic and strain-tunable two dimensional penta-X₂C family as water splitting photocatalysts with high carrier mobility. Journal of Materials Chemistry A, 2019, 7, 7791-7799.	10.3	66
4	Mechanism analysis of a flexible organic memristive memory with capacitance effect and negative differential resistance state. APL Materials, 2019, 7, .	5.1	51
5	Nanorod Array of SnO₂ Quantum Dot Interspersed Multiphase TiO₂ Heterojunctions with Highly Photocatalytic Water Splitting and Self-Rechargeable Battery-Like Applications. ACS Applied Materials & Interfaces, 2019, 11, 2071-2081.	8.0	48
6	Novel triadius-like N4 specie of iron nitride compounds under high pressure. Scientific Reports, 2018, 8, 10670.	3.3	36
7	Identifying the Ground-State NP Sheet through a Global Structure Search in Two-Dimensional Space and Its Promising High-Efficiency Photovoltaic Properties. , 2019, 1, 375-382.		26
8	Solar Cells Based on Two-Dimensional WTe₂/PtXY (X, Y = S, Se) Heterostructures with High Photoelectric Conversion Efficiency and Low Power Consumption. ACS Applied Energy Materials, 2021, 4, 357-364.	5.1	25
9	XTe (X = Ge, Sn, Pb) Monolayers: Promising Thermoelectric Materials with Ultralow Lattice Thermal Conductivity and High-power Factor. ES Energy & Environments, 2020, , .	1.1	25
10	Multiscale Modeling of Heat Dissipation in 2D Transistors Based on Phosphorene and Silicene. Journal of Physical Chemistry C, 2018, 122, 2641-2647.	3.1	24
11	Screw dislocation induced phonon transport suppression in SiGe superlattices. Physical Review B, 2019, 100, .	3.2	23
12	Elastic loading enhanced NH3 sensing for surface acoustic wave sensor with highly porous nitrogen doped diamond like carbon film. Sensors and Actuators B: Chemical, 2021, 344, 130175.	7.8	22
13	A novel 2D porous C₃N₂ framework as a promising anode material with ultra-high specific capacity for lithium-ion batteries. Journal of Materials Chemistry A, 2022, 10, 6551-6559.	10.3	22
14	Impeded thermal transport in composition graded SiGe nanowires. Applied Physics Letters, 2017, 111, .	3.3	21
15	Chemical kinetics of H-abstractions from dimethyl amine by H, CH₃, OH, and HO₂ radicals with multi-structural torsional anharmonicity. Physical Chemistry Chemical Physics, 2019, 21, 12685-12696.	2.8	21
16	Prediction and characterization of the marcasite phase of iron pernitride under high pressure. Journal of Alloys and Compounds, 2017, 702, 132-137.	5.5	20
17	Novel phonon resonator based on surface screw thread for suppressing thermal transport of Si nanowires. Physical Review B, 2020, 101, .	3.2	16
18	Exploring ion migration in Li₂MnSiO₄ for Li-ion batteries through strain effects. RSC Advances, 2017, 7, 26089-26096.	3.6	15

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19	Pressure induced evolution of structures and properties of iron tetraboride. CrystEngComm, 2018, 20, 3928-3935.	2.6	14
20	Benchmarking dual-level MS-Tor and DLPNO-CCSD(T) methods for H-abstraction from methyl pentanoate by an OH radical. Physical Chemistry Chemical Physics, 2019, 21, 20857-20867.	2.8	14
21	High-pressure induced phase transition of FeS2: Electronic, mechanical and thermoelectric properties. Journal of Alloys and Compounds, 2017, 710, 267-273.	5.5	13
22	Description of noncovalent interactions involving Ï€â€system with high precision: An assessment of RPA, MP2, and DFTâ€Đ methods. Journal of Computational Chemistry, 2019, 40, 1643-1651.	3.3	13
23	First-principles calculations of phonon transport in two-dimensional penta-X2C family. Journal of Applied Physics, 2020, 127, 205106.	2.5	13
24	Ultrahigh-pressure induced decomposition of silicon disulfide into silicon-sulfur compounds with high coordination numbers. Physical Review B, 2019, 99, .	3.2	10
25	Firstâ€Principles Study of Metal Atoms Adsorption on 2D Dumbbell C₄N. Physica Status Solidi (B): Basic Research, 2020, 257, 1900205.	1.5	9
26	Thermal decomposition mechanisms of LLM-105/HTPB plastic-bonded explosive: ReaxFF-lg molecular dynamics simulations. Journal of Energetic Materials, 2023, 41, 269-290.	2.0	9
27	Exploring the structures and properties of nickel silicides at the pressures of the Earthâ€™s core. Physical Chemistry Chemical Physics, 2021, 23, 14671-14677.	2.8	8
28	The thermoelectric properties of Î±-XP (X = Sb and Bi) monolayers from first-principles calculations. Physical Chemistry Chemical Physics, 2021, 23, 24598-24606.	2.8	8
29	Tunable Electronic Properties and Potential Applications of BSe/XS₂ (X=Mo, W) van der Waals Heterostructures. Advanced Theory and Simulations, 2020, 3, 2000144.	2.8	7
30	2D auxetic material with intrinsic ferromagnetism: a copper halide (CuCl₂) monolayer. Physical Chemistry Chemical Physics, 2021, 23, 22078-22085.	2.8	7
31	Ultralow lattice thermal conductivity and high thermoelectric performance of penta-Sb2C monolayer: A first principles study. Journal of Applied Physics, 2021, 130, 185104.	2.5	7
32	Pressure induced structural phase of lithium disulfide with a close to intermediate product character of lithium-sulfur battery. Journal of Alloys and Compounds, 2019, 778, 588-592.	5.5	6
33	Strain-tuned mechanical, electronic, and optoelectronic properties of two-dimensional transition metal sulfides ZrS2: a first-principles study. Journal of Molecular Modeling, 2022, 28, 63.	1.8	5
34	Exploring Molecules beyond CO as Tip Functionalizations in High-Resolution Noncontact Atomic Force Microscopy: A First Principles Approach. ACS Omega, 2016, 1, 1004-1009.	3.5	4
35	High pressure induced decomposition of antimony trisulfide. Materials Today Communications, 2021, 29, 102828.	1.9	3
36	DFT calculations of the structures, electronic and spectral properties for FenSm (2 â‰¤ n + m â‰¤ 5) clusters. European Physical Journal D, 2019, 73, 1.	1.3	2

#	Article	IF	Citations
37	Design and modulation of two-dimensional Dirac materials in beryllium/boron-based binary monolayers. Computational Materials Science, 2021, 199, 110727.	3.0	2
38	Promising thermoelectric candidate based on a CaAs₃ monolayer: A first principles study. Physical Chemistry Chemical Physics, 2021, 23, 24039-24046.	2.8	2