

# Hongyan Wang

## List of Publications by Year in descending order

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38  
papers

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citations

516710

16  
h-index

501196

28  
g-index

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38  
docs citations

38  
times ranked

1024  
citing authors

| #  | ARTICLE  | IF   | CITATIONS |
|----|--|------|-----------|
| 1  | Thermal decomposition mechanisms of LLM-105/HTPB plastic-bonded explosive: ReaxFF-Ig molecular dynamics simulations. <i>Journal of Energetic Materials</i> , 2023, 41, 269-290.  | 2.0  | 9         |
| 2  | A novel 2D porous C <sub>3</sub> N <sub>2</sub> framework as a promising anode material with ultra-high specific capacity for lithium-ion batteries. <i>Journal of Materials Chemistry A</i> , 2022, 10, 6551-6559.          | 10.3 | 22        |
| 3  | Strain-tuned mechanical, electronic, and optoelectronic properties of two-dimensional transition metal sulfides ZrS <sub>2</sub> : a first-principles study. <i>Journal of Molecular Modeling</i> , 2022, 28, 63.            | 1.8  | 5         |
| 4  | 2D auxetic material with intrinsic ferromagnetism: a copper halide (CuCl <sub>2</sub> ) monolayer. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22078-22085.   | 2.8  | 7         |
| 5  | High pressure induced decomposition of antimony trisulfide. <i>Materials Today Communications</i> , 2021, 29, 102828.  | 1.9  | 3         |
| 6  | Elastic loading enhanced NH <sub>3</sub> sensing for surface acoustic wave sensor with highly porous nitrogen doped diamond like carbon film. <i>Sensors and Actuators B: Chemical</i> , 2021, 344, 130175.                  | 7.8  | 22        |
| 7  | Design and modulation of two-dimensional Dirac materials in beryllium/boron-based binary monolayers. <i>Computational Materials Science</i> , 2021, 199, 110727.   | 3.0  | 2         |
| 8  | Exploring the structures and properties of nickel silicides at the pressures of the Earth's core. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14671-14677.  | 2.8  | 8         |
| 9  | Solar Cells Based on Two-Dimensional WTe <sub>2</sub> /PtXY (X, Y = S, Se) Heterostructures with High Photoelectric Conversion Efficiency and Low Power Consumption. <i>ACS Applied Energy Materials</i> , 2021, 4, 357-364. | 5.1  | 25        |
| 10 | The thermoelectric properties of $\hat{\Gamma}$ -XP (X = Sb and Bi) monolayers from first-principles calculations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24598-24606.                                       | 2.8  | 8         |
| 11 | Promising thermoelectric candidate based on a CaAs <sub>3</sub> monolayer: A first principles study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 24039-24046.   | 2.8  | 2         |
| 12 | Ultralow lattice thermal conductivity and high thermoelectric performance of penta-Sb <sub>2</sub> C monolayer: A first principles study. <i>Journal of Applied Physics</i> , 2021, 130, 185104.                             | 2.5  | 7         |
| 13 | First-Principles Study of Metal Atoms Adsorption on 2D Dumbbell C <sub>4</sub> N. <i>Physica Status Solidi (B): Basic Research</i> , 2020, 257, 1900205.   | 1.5  | 9         |
| 14 | Tunable Electronic Properties and Potential Applications of BSe/XS <sub>2</sub> (X=Mo, W) van der Waals Heterostructures. <i>Advanced Theory and Simulations</i> , 2020, 3, 2000144.   | 2.8  | 7         |
| 15 | Novel phonon resonator based on surface screw thread for suppressing thermal transport of Si nanowires. <i>Physical Review B</i> , 2020, 101, .  | 3.2  | 16        |
| 16 | First-principles calculations of phonon transport in two-dimensional penta-X <sub>2</sub> C family. <i>Journal of Applied Physics</i> , 2020, 127, 205106.   | 2.5  | 13        |
| 17 | XTe (X = Ge, Sn, Pb) Monolayers: Promising Thermoelectric Materials with Ultralow Lattice Thermal Conductivity and High-power Factor. <i>ES Energy &amp; Environments</i> , 2020, , .  | 1.1  | 25        |
| 18 | Mechanism analysis of a flexible organic memristive memory with capacitance effect and negative differential resistance state. <i>APL Materials</i> , 2019, 7, .   | 5.1  | 51        |

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|----|---|------|-----------|
| 19 | 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        |
| 20 | Screw dislocation induced phonon transport suppression in SiGe superlattices. Physical Review B, 2019, 100, .   | 3.2  | 23        |
| 21 | 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        |
| 22 | Chemical kinetics of H-abstractions from dimethyl amine by H, CH <sub>3</sub> , OH, and HO <sub>2</sub> radicals with multi-structural torsional anharmonicity. Physical Chemistry Chemical Physics, 2019, 21, 12685-12696.                                 | 2.8  | 21        |
| 23 | Ultrahigh-pressure induced decomposition of silicon disulfide into silicon-sulfur compounds with high coordination numbers. Physical Review B, 2019, 99, .  | 3.2  | 10        |
| 24 | DFT calculations of the structures, electronic and spectral properties for FenSm (2 ≤ n + m ≤ 5) clusters. European Physical Journal D, 2019, 73, 1.  | 1.3  | 2         |
| 25 | Flexible, auxetic and strain-tunable two dimensional penta-X <sub>2</sub> C family as water splitting photocatalysts with high carrier mobility. Journal of Materials Chemistry A, 2019, 7, 7791-7799.  | 10.3 | 66        |
| 26 | 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        |
| 27 | Description of noncovalent interactions involving ĩ€€system with high precision: An assessment of RPA, MP2, and DFT methods. Journal of Computational Chemistry, 2019, 40, 1643-1651.   | 3.3  | 13        |
| 28 | Nanorod Array of SnO <sub>2</sub> Quantum Dot Interspersed Multiphase TiO <sub>2</sub> Heterojunctions with Highly Photocatalytic Water Splitting and Self-Rechargeable Battery-Like Applications. ACS Applied Materials & Interfaces, 2019, 11, 2071-2081. | 8.0  | 48        |
| 29 | 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         |
| 30 | 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        |
| 31 | Novel two-dimensional semiconductor SnP <sub>3</sub> : 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       |
| 32 | Pressure induced evolution of structures and properties of iron tetraboride. CrystEngComm, 2018, 20, 3928-3935.   | 2.6  | 14        |
| 33 | Novel triadius-like N4 specie of iron nitride compounds under high pressure. Scientific Reports, 2018, 8, 10670.  | 3.3  | 36        |
| 34 | 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        |
| 35 | Exploring ion migration in Li <sub>2</sub> MnSiO <sub>4</sub> for Li-ion batteries through strain effects. RSC Advances, 2017, 7, 26089-26096.  | 3.6  | 15        |
| 36 | High-pressure induced phase transition of FeS <sub>2</sub> : Electronic, mechanical and thermoelectric properties. Journal of Alloys and Compounds, 2017, 710, 267-273.   | 5.5  | 13        |

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|----|--|-----|-----------|
| 37 | Impeded thermal transport in composition graded SiGe nanowires. <i>Applied Physics Letters</i> , 2017, 111, .  | 3.3 | 21        |
| 38 | Exploring Molecules beyond CO as Tip Functionalizations in High-Resolution Noncontact Atomic Force Microscopy: A First Principles Approach. <i>ACS Omega</i> , 2016, 1, 1004-1009. | 3.5 | 4         |