Junjie Wang

List of Publications by Year
in descending order

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51 papers	2,414 citations	257101 24 h-index	205818 48 g-index
54 all docs	54 docs citations	54 times ranked	3430 citing authors

#	Article	IF	Citations
1	Surfaceâ€Plasmonâ€Enhanced Photodriven CO₂ Reduction Catalyzed by Metalâ€“Organicâ€Frameworkâ€Derived Iron Nanoparticles Encapsulated by Ultrathin Carbon Layers. Advanced Materials, 2016, 28, 3703-3710.	11.1	300
2	Ternary intermetallic LaCoSi as a catalyst for N2 activation. Nature Catalysis, 2018, 1, 178-185.	16.1	221
3	Discovery of hexagonal ternary phase Ti2InB2 and its evolution to layered boride TiB. Nature Communications, 2019, 10, 2284.	5.8	159
4	Photocatalytic Water Splitting under Visible Light by Mixed-Valence Sn₃O₄. ACS Applied Materials & Interfaces, 2014, 6, 3790-3793.	4.0	148
5	First-principles study of the relaxation and energy of bcc-Fe, fcc-Fe and AISI-304 stainless steel surfaces. Applied Surface Science, 2009, 255, 9032-9039.	3.1	120
6	Novel MAB phases and insights into their exfoliation into 2D MBenes. Nanoscale, 2019, 11, 11305-11314.	2.8	120
7	Mesoporous palladiumâ€“copper bimetallic electrodes for selective electrocatalytic reduction of aqueous CO₂to CO. Journal of Materials Chemistry A, 2016, 4, 4776-4782.	5.2	115
8	Computational Prediction of Boron-Based MAX Phases and MXene Derivatives. Chemistry of Materials, 2020, 32, 6947-6957.	3.2	89
9	Tiered Electron Anions in Multiple Voids of LaScSi and Their Applications to Ammonia Synthesis. Advanced Materials, 2017, 29, 1700924.	11.1	85
10	Exploration of Stable Strontium Phosphide-Based Electrides: Theoretical Structure Prediction and Experimental Validation. Journal of the American Chemical Society, 2017, 139, 15668-15680.	6.6	84
11	Determination of Crystal Structure of Graphitic Carbon Nitride: Ab Initio Evolutionary Search and Experimental Validation. Chemistry of Materials, 2017, 29, 2694-2707.	3.2	83
12	Crystal structure and elastic properties of ZrB compared with ZrB2: A first-principles study. Computational Materials Science, 2010, 49, 814-819.	1.4	79
13	Mixed Valence Tin Oxides as Novel van der Waals Materials: Theoretical Predictions and Potential Applications. Advanced Energy Materials, 2016, 6, 1501190.	10.2	79
14	Influence of laser deposition patterns on part distortion, interior quality and mechanical properties by laser solid forming (LSF). Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2011, 528, 1094-1104.	2.6	65
15	Two-Dimensional GeSe as an Isostructural and Isoelectronic Analogue of Phosphorene: Sonication-Assisted Synthesis, Chemical Stability, and Optical Properties. Chemistry of Materials, 2017, 29, 8361-8368.	3.2	65
16	Semimetallic Two-Dimensional TiB₁₂: Improved Stability and Electronic Properties Tunable by Biaxial Strain. Chemistry of Materials, 2017, 29, 5922-5930.	3.2	41
17	Adsorption of atomic and molecular oxygen on SiC-Si(111) and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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19	Mechanics and energy analysis on molten pool spreading during laser solid forming. Applied Surface Science, 2010, 256, 4612-4620.	3.1	37
20	Theoretical Investigation for the Activeâ€toâ€Passive Transition in the Oxidation of Silicon Carbide. Journal of the American Ceramic Society, 2008, 91, 1665-1673.	1.9	35
21	Discovery of stable and intrinsic antiferromagnetic iron oxyhalide monolayers. Physical Chemistry Chemical Physics, 2020, 22, 11731-11739.	1.3	32
22	Discovery of intrinsic two-dimensional antiferromagnets from transition-metal borides. Nanoscale, 2021, 13, 8254-8263.	2.8	31
23	Realization of Mott-Insulating electrides in dimorphic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">Y</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>5</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:msub><mml:mi mathvariant="normal">b</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physi	1.1	30
24	Ternary inorganic electrides with mixed bonding. Physical Review B, 2019, 99, .	1.1	26
25	Surface relaxation and oxygen adsorption behavior of different SiC polytypes: a first-principles study. Journal of Physics Condensed Matter, 2010, 22, 265003.	0.7	22
26	Electron-Deficient-Type Electride Ca₅Pb₃: Extension of Electride Chemical Space. Journal of the American Chemical Society, 2021, 143, 8821-8828.	6.6	22
27	Exploring structural, electronic, and mechanical properties of 2D hexagonal MBenes. Journal of Physics Condensed Matter, 2021, 33, 155503.	0.7	20
28	Unraveling the size-dependent effect of Ru-based catalysts on Ammonia synthesis at mild conditions. Journal of Catalysis, 2021, 404, 501-511.	3.1	20
29	Hexagonal MBene (Hf₂BO₂): A Promising Platform for the Electrocatalysis of Hydrogen Evolution Reaction. ACS Applied Materials & Interfaces, 2021, 13, 56131-56139.	4.0	20
30	LaRuSi Electride Disrupts the Scaling Relations for Ammonia Synthesis. Chemistry of Materials, 2022, 34, 1677-1685.	3.2	19
31	Hypercoordinate two-dimensional transition-metal borides for spintronics and catalyst applications. Journal of Materials Chemistry C, 0, , .	2.7	18
32	B₅N₃ and B₇N₅ Monolayers with High Carrier Mobility and Excellent Optical Performance. Journal of Physical Chemistry Letters, 2021, 12, 4823-4832.	2.1	18
33	First-principles investigation on initial stage of 2H-SiC(001) surface oxidation. Science Bulletin, 2009, 54, 1487-1494.	4.3	17
34	Theoretical exploration of quaternary hexagonal MAB phases and two-dimensional derivatives. Nanoscale, 2021, 13, 13208-13214.	2.8	16
35	Evolutionary structure prediction of two-dimensional IrB₁₄: a promising gas sensor material. Journal of Materials Chemistry C, 2018, 6, 5803-5811.	2.7	13
36	The rate-limiting step in the thermal oxidation of silicon carbide. Scripta Materialia, 2010, 62, 654-657.	2.6	12

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37	A-Site Cation Bulk and Surface Diffusion in A-Site-Deficient BaZrO₃ and SrZrO₃ Perovskites. Journal of Physical Chemistry C, 2017, 121, 12220-12229.	1.5	11
38	Design of p-type transparent conducting oxides Sn₂GeO₄ by an ab initio evolutionary structure search. Journal of Materials Chemistry C, 2018, 6, 11202-11208.	2.7	11
39	Crystal and electronic structure engineering of tin monoxide by external pressure. Journal of Advanced Ceramics, 2021, 10, 565-577.	8.9	11
40	Discovery of Electrides in Electronâ€Rich Nonâ€Electride Materials via Energy Modification of Interstitial Electrons. Advanced Functional Materials, 2022, 32, .	7.8	8
41	Germanium Adsorption and Initial Growth on SrTiO₃(001) Surface: A First-Principles Investigation. Journal of Physical Chemistry C, 2011, 115, 22893-22900.	1.5	7
42	First Principles Evolutionary Search for New Electrides along the Dimensionality of Anionic Electrons. Journal of Computer Chemistry Japan, 2017, 16, 135-138.	0.0	6
43	High-Pressure Phase Diagram of the Tiâ€“O System. Journal of Physical Chemistry Letters, 2021, 12, 5486-5493.	2.1	5
44	Molecular dynamics study of pyrolytic carbon interphase in CF/CIpreform. Modelling and Simulation in Materials Science and Engineering, 2003, 11, 897-904.	0.8	4
45	Prediction of allotropes of tellurium with molecular, one- and two-dimensional covalent nets for photofunctional applications. RSC Advances, 2021, 11, 29965-29975.	1.7	4
46	Mining Knowledge from Crystal Structures: Oxidation States of Oxygen-Coordinated Metal Atoms in Ionic and Coordination Compounds. Journal of Chemical Information and Modeling, 2022, 62, 2332-2340.	2.5	4
47	Phase diagram exploration of Tcâ€“Alâ€“B: from bulk Tc₂AlB₂ to two-dimensional Tc₂B₂. Physical Chemistry Chemical Physics, 2021, 23, 22086-22095.	1.3	3
48	Modified Wagner model for the active-to-passive transition in the oxidation of Si₃N₄. Journal Physics D: Applied Physics, 2008, 41, 115412.	1.3	1
49	Germanium Growth Orientation on SrTiO3 (001) 2 Ã— 1 Surface: Role of Surface Reduction. Journal of Physical Chemistry C, 2013, 117, 9887-9894.	1.5	1
50	Chapter 2. Theoretical Design of PEC Materials. RSC Energy and Environment Series, 2018, , 29-61.	0.2	1
51	Photocatalysis and hydrogen production from water solution. , 2020, , 555-577.		0