Wujie Qiu

List of Publications by Year in descending order

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44 papers	1,714 citations	471509 17 h-index	276875 41 g-index
44 all docs	44 docs citations	44 times ranked	2439 citing authors

#	Article	IF	Citations
1	On the tuning of electrical and thermal transport in thermoelectrics: an integrated theoryâ€“experiment perspective. Npj Computational Materials, 2016, 2, .	8.7	399
2	Part-crystalline part-liquid state and rattling-like thermal damping in materials with chemical-bond hierarchy. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 15031-15035.	7.1	225
3	Adsorption-energy-based activity descriptors for electrocatalysts in energy storage applications. National Science Review, 2018, 5, 327-341.	9.5	129
4	Silicene: Wetâ€Chemical Exfoliation Synthesis and Biodegradable Tumor Nanomedicine. Advanced Materials, 2019, 31, e1903013.	21.0	112
5	Auto-optimizing Hydrogen Evolution Catalytic Activity of ReS₂ through Intrinsic Charge Engineering. ACS Nano, 2018, 12, 4486-4493.	14.6	111
6	Multiformity and fluctuation of Cu ordering in Cu₂Se thermoelectric materials. Journal of Materials Chemistry A, 2015, 3, 6901-6908.	10.3	80
7	Significant Roles of Intrinsic Point Defects in Mg₂X (X = Si, Ge, Sn) Thermoelectric Materials. Advanced Electronic Materials, 2016, 2, 1500284.	5.1	75
8	Diverse lattice dynamics in ternary Cu-Sb-Se compounds. Scientific Reports, 2015, 5, 13643.	3.3	51
9	Bond Electronegativity as Hydrogen Evolution Reaction Catalyst Descriptor for Transition Metal (TM) Tj ETQq1 1 0.784314 rgBT /Ove	6.7	45
10	Identifying Metallic Transition-Metal Dichalcogenides for Hydrogen Evolution through Multilevel High-Throughput Calculations and Machine Learning. Journal of Physical Chemistry Letters, 2021, 12, 2102-2111.	4.6	43
11	Intrinsically low thermal conductivity from a quasi-one-dimensional crystal structure and enhanced electrical conductivity network via Pb doping in SbCrSe3. NPG Asia Materials, 2017, 9, e387-e387.	7.9	37
12	Structure family and polymorphous phase transition in the compounds with soft sublattice: Cu2Se as an example. Journal of Chemical Physics, 2016, 144, 194502.	3.0	35
13	Reducing the charge overpotential of Liâ€“O₂ batteries through band-alignment cathode design. Energy and Environmental Science, 2020, 13, 2540-2548.	30.8	30
14	Recent progress in theoretical and computational investigations of structural stability and activity of single-atom electrocatalysts. Progress in Natural Science: Materials International, 2019, 29, 256-264.	4.4	27
15	Thermoelectric materials with crystal-amorphicity duality induced by large atomic size mismatch. Joule, 2021, 5, 1183-1195.	24.0	27
16	Hydrogen-bonded silicene nanosheets of engineered bandgap and selective degradability for photodynamic therapy. Biomaterials, 2021, 278, 121172.	11.4	21
17	Novel meta-phase arising from large atomic size mismatch. Matter, 2022, 5, 605-615.	10.0	20
18	Water-Enabled H₂ Generation from Hydrogenated Silicon Nanosheets for Efficient Anti-Inflammation. Journal of the American Chemical Society, 2022, 144, 14195-14206.	13.7	18

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19	Polytypism in superhard transition-metal triborides. Scientific Reports, 2014, 4, 5063.	3.3	17
20	A new phase of ThC at high pressure predicted from a first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 1607-1611.	2.1	17
21	Tight bonding and high-efficiency utilization of Sâ€“S moieties to enable ultra-stable and high-capacity alkali-metal conversion batteries. Journal of Materials Chemistry A, 2021, 9, 6160-6171.	10.3	17
22	How inactive d0 transition metal controls anionic redox in disordered Li-rich oxyfluoride cathodes. Energy Storage Materials, 2020, 32, 253-260.	18.0	16
23	Stabilizing Low-Coordinated O Ions To Operate Cationic and Anionic Redox Chemistry of Li-Ion Battery Materials. ACS Applied Materials & Interfaces, 2019, 11, 37768-37778.	8.0	13
24	Superposed Redox Chemistry of Fused Carbon Rings in Cyclooctatetraene-Based Organic Molecules for High-Voltage and High-Capacity Cathodes. ACS Applied Materials & Interfaces, 2018, 10, 2496-2503.	8.0	12
25	Partial Disproportionation Gallium-Oxygen Reaction Boosts Lithium-Oxygen Batteries. Energy Storage Materials, 2021, 41, 475-484.	18.0	12
26	Structural and electronic phase transitions of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ThS</mml:mi><mml:mn>2</mml:mn></mml:msub></mm first-principles calculations. Physical Review B, 2016, 94, .	3.2	11
27	The orderâ€“disorder transition in Cu₂Se and medium-range ordering in the high-temperature phase. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 201-207.	1.1	11
28	Lattice dynamics and lattice thermal conductivity of thorium dicarbide. Journal of Nuclear Materials, 2014, 454, 142-148.	2.7	10
29	Dynamic process of the resonant phonon scattering in fully filled skutterudites. Physical Review B, 2018, 98, .	3.2	10
30	Cooperative Effect of Multiple Active Sites and Hierarchical Chemical Bonds in Metalâ€“Organic Compounds for Improving Cathode Performance. ACS Energy Letters, 2020, 5, 477-485.	17.4	10
31	Alkaline-earth metal substitution stabilizes the anionic redox of Li-rich oxides. Journal of Materials Chemistry A, 2021, 9, 10364-10373.	10.3	10
32	The critical role of oxygen-evolution kinetics in the electrochemical stability of oxide superionic conductors. Journal of Materials Chemistry A, 2019, 7, 17008-17013.	10.3	8
33	Vacancy-induced anion and cation redox chemistry in cation-deficient F-doped anatase TiO2. Journal of Materials Chemistry A, 2020, 8, 20393-20401.	10.3	8
34	Enhanced Thermoelectric Performance in Ge_{0.955â˜}_xSb_xTe/FeGe₂ Composites Enabled by Hierarchical Defects. Small, 2021, 17, e2100915.	10.0	8
35	â€œPhononâ€•scattering beyond perturbation theory. Science China: Physics, Mechanics and Astronomy, 2016, 59, 1.	5.1	6
36	Multiscale computations and artificial intelligent models of electrochemical performance in Liâ€‐ion battery materials. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	6

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37	Predicting Transitionâ€Metal/Benzenehexathiol Systems as Effective Cathodes of Liâ€S batteries with Conjugate Conductivity and Synergetic Discharge. ChemistrySelect, 2020, 5, 7783-7788.	1.5	5
38	Predicting Li-Rich Layered Oxide Compounds as High-Conductivity and Stable Solid Electrolytes. ACS Energy Letters, 2021, 6, 3793-3800.	17.4	5
39	Origin of multiple voltage plateaus in P2-type sodium layered oxides. Materials Horizons, 2022, 9, 1460-1467.	12.2	5
40	Structural phase transitions and superconductivity of YC2 from first-principles calculations. Computational Materials Science, 2019, 159, 120-126.	3.0	4
41	Kinetics of bonds at structural breakdown in boron carbide under intensive loads: A molecular dynamics study. Computational Materials Science, 2020, 180, 109711.	3.0	4
42	Electrochemical Activity of Positive Electrode Material of P2-Na_x[Mg_{0.33}Mn_{0.67}]O₂ Sodium Ion Battery. Wuji Cailiao Xuebao/Journal of Inorganic Materials, 2021, 36, 623.	1.3	3
43	Thermal transport and microscopic dynamics in filled skutterudite YbFe4Sb12 studied by ab initio molecular dynamics simulation. Wuli Xuebao/Acta Physica Sinica, 2018, 67, 016301.	0.5	1
44	Preparation and characterization of orthorhombic Fe2(MoO4)3 and first-principle study of its negative thermal expansion properties. Wuli Xuebao/Acta Physica Sinica, 2016, 65, 056501.	0.5	0