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	Novel meta-phase arising from large atomic size mismatch. Matter, 2022, 5, 605-615.	10.0	20
2	Origin of multiple voltage plateaus in P2-type sodium layered oxides. Materials Horizons, 2022, 9, 1460-1467.	12.2	5
3	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
4	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
5	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
6	Alkaline-earth metal substitution stabilizes the anionic redox of Li-rich oxides. Journal of Materials Chemistry A, 2021, 9, 10364-10373.	10.3	10
7	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
8	Enhanced Thermoelectric Performance in Ge_{0.955â˜}_xSb_xTe/FeGe₂ Composites Enabled by Hierarchical Defects. Small, 2021, 17, e2100915.	10.0	8
9	Thermoelectric materials with crystal-amorphicity duality induced by large atomic size mismatch. Joule, 2021, 5, 1183-1195.	24.0	27
10	Partial Disproportionation Gallium-Oxygen Reaction Boosts Lithium-Oxygen Batteries. Energy Storage Materials, 2021, 41, 475-484.	18.0	12
11	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
12	Predicting Li-Rich Layered Oxide Compounds as High-Conductivity and Stable Solid Electrolytes. ACS Energy Letters, 2021, 6, 3793-3800.	17.4	5
13	Hydrogen-bonded silicene nanosheets of engineered bandgap and selective degradability for photodynamic therapy. Biomaterials, 2021, 278, 121172.	11.4	21
14	Bond Electronegativity as Hydrogen Evolution Reaction Catalyst Descriptor for Transition Metal (TM) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	6.7	45
15	How inactive d0 transition metal controls anionic redox in disordered Li-rich oxyfluoride cathodes. Energy Storage Materials, 2020, 32, 253-260.	18.0	16
16	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
17	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
18	Reducing the charge overpotential of Liâ€“O₂ batteries through band-alignment cathode design. Energy and Environmental Science, 2020, 13, 2540-2548.	30.8	30

#	Article	IF	Citations
19	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
20	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
21	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
22	Silicene: Wetâ€Chemical Exfoliation Synthesis and Biodegradable Tumor Nanomedicine. Advanced Materials, 2019, 31, e1903013.	21.0	112
23	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
24	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
25	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
26	Structural phase transitions and superconductivity of YC2 from first-principles calculations. Computational Materials Science, 2019, 159, 120-126.	3.0	4
27	Adsorption-energy-based activity descriptors for electrocatalysts in energy storage applications. National Science Review, 2018, 5, 327-341.	9.5	129
28	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
29	Auto-optimizing Hydrogen Evolution Catalytic Activity of ReS₂ through Intrinsic Charge Engineering. ACS Nano, 2018, 12, 4486-4493.	14.6	111
30	Dynamic process of the resonant phonon scattering in fully filled skutterudites. Physical Review B, 2018, 98, .	3.2	10
31	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
32	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
33	Significant Roles of Intrinsic Point Defects in Mg₂X (X = Si, Ge, Sn) Thermoelectric Materials. Advanced Electronic Materials, 2016, 2, 1500284.	5.1	75
34	On the tuning of electrical and thermal transport in thermoelectrics: an integrated theoryâ€“experiment perspective. Npj Computational Materials, 2016, 2, .	8.7	399
35	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
36	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

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37	â€œPhononâ€•scattering beyond perturbation theory. Science China: Physics, Mechanics and Astronomy, 2016, 59, 1.	5.1	6
38	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
39	Diverse lattice dynamics in ternary Cu-Sb-Se compounds. Scientific Reports, 2015, 5, 13643.	3.3	51
40	Multiformity and fluctuation of Cu ordering in Cu₂Se thermoelectric materials. Journal of Materials Chemistry A, 2015, 3, 6901-6908.	10.3	80
41	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
42	Lattice dynamics and lattice thermal conductivity of thorium dicarbide. Journal of Nuclear Materials, 2014, 454, 142-148.	2.7	10
43	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
44	Polytypism in superhard transition-metal triborides. Scientific Reports, 2014, 4, 5063.	3.3	17