Wei-Hua Wang

List of Publications by Year
in descending order

60 papers	2,311 citations	331670 21 h-index	214800 47 g-index
62 all docs	62 docs citations	62 times ranked	4564 citing authors

#	Article	IF	Citations
1	Band alignment of two-dimensional transition metal dichalcogenides: Application in tunnel field effect transistors. Applied Physics Letters, 2013, 103, .	3.3	657
2	First Principles Calculations of Electronic Band Structure and Optical Properties of Cr-Doped ZnO. Journal of Physical Chemistry C, 2009, 113, 8460-8464.	3.1	229
3	A Semiâ€Conductive Copperâ€"Organic Framework with Two Types of Photocatalytic Activity. Angewandte Chemie - International Edition, 2016, 55, 4938-4942.	13.8	164
4	Systematic study of electronic structure and band alignment of monolayer transition metal dichalcogenides in Van der Waals heterostructures. 2D Materials, 2017, 4, 015026.	4.4	160
5	Ab initio study of doping effects on LiMnO₂ and Li₂MnO₃ cathode materials for Li-ion batteries. Journal of Materials Chemistry A, 2015, 3, 8489-8500.	10.3	102
6	Electric-field control of ferromagnetism through oxygen ion gating. Nature Communications, 2017, 8, 2156.	12.8	85
7	Zinc-Blende CdS Nanocubes with Coordinated Facets for Photocatalytic Water Splitting. ACS Catalysis, 2017, 7, 1470-1477.	11.2	83
8	Surface plasmon resonance enhanced visible-light-driven photocatalytic activity in Cu nanoparticles covered Cu2O microspheres for degrading organic pollutants. Applied Surface Science, 2016, 366, 120-128.	6.1	64
9	Two-Dimensional Superlattice: Modulation of Band Gaps in Graphene-Based Monolayer Carbon Superlattices. Journal of Physical Chemistry Letters, 2012, 3, 3373-3378.	4.6	60
10	Electronic structures, magnetic properties and band alignments of 3d transition metal atoms doped monolayer MoS2. Physics Letters, Section A: General, Atomic and Solid State Physics, 2018, 382, 111-115.	2.1	51
11	A class of monolayer metal halogenides MX2: Electronic structures and band alignments. Applied Physics Letters, 2016, 108, .	3.3	49
12	Electronic structures and band alignments of monolayer metal trihalide semiconductors MX₃. Journal of Materials Chemistry C, 2017, 5, 9066-9071.	5.5	45
13	Identifying the descriptor governing NO oxidation on mullite Sm(Y, Tb, Gd,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 267 Td (Lu)M 2016, 6, 3971-3975.	4.1	44
14	Schottky Barrier Height of Pd/MoS₂ Contact by Large Area Photoemission Spectroscopy. ACS Applied Materials & Interfaces, 2017, 9, 38977-38983.	8.0	36
15	A Spatially Separated Organicâ€"Inorganic Hybrid Photoelectrochemical Cell for Unassisted Overall Water Splitting. ACS Catalysis, 2017, 7, 5308-5315.	11.2	33
16	Efficient photo-degradation of dyes using CuWO₄ nanoparticles with electron sacrificial agents: a combination of experimental and theoretical exploration. RSC Advances, 2016, 6, 953-959.	3.6	29
17	Origin of Indium Diffusion in High-<i>k</i> Oxide HfO₂. ACS Applied Materials & Interfaces, 2016, 8, 7595-7600.	8.0	28
18	TiO₂â€"P3HT:PCBM photoelectrochemical tandem cells for solar-driven overall water splitting. Journal of Materials Chemistry A, 2018, 6, 4032-4039.	10.3	28

#	Article	IF	Citations
19	Electronic properties and native point defects of high efficient NO oxidation catalysts SmMn2O5. Applied Physics Letters, 2016, 109, .	3.3	27
20	Origin of theoretical pseudocapacitance of two-dimensional supercapacitor electrodes Ti₃C₂T₂ (T = bare, O, S). Journal of Materials Chemistry A, 2019, 7, 16231-16238.	10.3	26
21	Magnetic borophenes from an evolutionary search. Physical Review B, 2019, 99, .	3.2	25
22	Metallic Monolayer Ta₂CS₂: An Anode Candidate for Li⁺, Na⁺, K⁺, and Ca²⁺ Ion Batteries. ACS Applied Energy Materials, 2020, 3, 10695-10701.	5.1	23
23	ITO regulated high-performance n-Si/ITO/Î±-Fe2O3 Z-scheme heterostructure towards photoelectrochemical water splitting. Journal of Catalysis, 2020, 381, 501-507.	6.2	20
24	A Semiâ€Conductive Copperâ€“Organic Framework with Two Types of Photocatalytic Activity. Angewandte Chemie, 2016, 128, 5022-5026.	2.0	19
25	First Principles Study of Tritium Diffusion in Li2TiO3 Crystal with Lithium Vacancy. Materials, 2018, 11, 2383.	2.9	16
26	Room-temperature ferromagnetism in nanocrystalline Cu/Cu2O core-shell structures prepared by magnetron sputtering. APL Materials, 2013, 1, .	5.1	15
27	Dehydration of Electrochemically Protonated Oxide: SrCoO₂ with Square Spin Tubes. Journal of the American Chemical Society, 2021, 143, 17517-17525.	13.7	15
28	Origin of OER catalytic activity difference of oxygen-deficient perovskites A2Mn2O5 (A = Ca, Sr): A theoretical study. Journal of Chemical Physics, 2017, 146, 224703.	3.0	12
29	Ideal two-dimensional molecular sieves for gas separation: Metal trihalides MX3 with precise atomic pores. Journal of Membrane Science, 2020, 602, 117786.	8.2	12
30	Ferroelectricâ€Like Behavior in TaN/Highâ€k/Si System Based on Amorphous Oxide. Advanced Electronic Materials, 2021, 7, 2100414.	5.1	12
31	First-Principles Study of Crown Ether and Crown Ether-Li Complex Interactions with Graphene. Journal of Physical Chemistry C, 2015, 119, 20016-20022.	3.1	11
32	High-throughput identification of one-dimensional atomic wires and first principles calculations of their electronic states*. Chinese Physics B, 2021, 30, 057304.	1.4	11
33	Electronic Structure and Ferromagnetism Modulation in Cu/Cu2O Interface: Impact of Interfacial Cu Vacancy and Its Diffusion. Scientific Reports, 2015, 5, 15191.	3.3	9
34	Energetics of metal ion adsorption on and diffusion through crown ethers: First principles study on two-dimensional electrolyte. Solid State Ionics, 2017, 301, 176-181.	2.7	9
35	Improved carrier doping strategy of monolayer MoS2 through two-dimensional solid electrolyte of YBr3. Applied Physics Letters, 2019, 114, .	3.3	9
36	Ideal two-dimensional solid electrolytes for fast ion transport: metal trihalides MX3 with intrinsic atomic pores. Nanoscale, 2020, 12, 7188-7195.	5.6	9

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37	Correlation effects in the electronic structure of the Ni-based superconducting KNi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>S<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 87, .	3.2	6
38	Elucidating dz2 orbital selective catalytic activity in brownmillerite Ca2Mn2O5. AIP Advances, 2016, 6, 095210.	1.3	6
39	Molecularly Thin Electrolyte for All Solid-State Nonvolatile Two-Dimensional Crystal Memory. Nano Letters, 2019, 19, 8911-8919.	9.1	6
40	Design rules of pseudocapacitive electrode materials: ion adsorption, diffusion, and electron transmission over prototype TiO2. Science China Materials, 2022, 65, 391-399.	6.3	6
41	Titanium Nitride Protected Cuprous Oxide Photocathode for Stable and Efficient Water Reduction. ACS Applied Energy Materials, 2022, 5, 770-776.	5.1	6
42	Synergistic synthesis of quasi-monocrystal CdS nanoboxes with high-energy facets. Journal of Materials Chemistry A, 2015, 3, 23106-23112.	10.3	5
43	Molecular dynamics simulations of interaction and very first step oxidation in the surface of ferritic Fe-Cr alloy. Computational Materials Science, 2021, 195, 110500.	3.0	5
44	Molecular dynamics simulations of the initial oxidation process on ferritic Feâ€“Cr alloy surfaces. RSC Advances, 2022, 12, 9501-9511.	3.6	5
45	Exploring the microscopic mechanism of pseudocapacitance with electronic structures in monolayer 1T-MoS₂ electrodes for supercapacitors. Materials Chemistry Frontiers, 2019, 3, 1310-1316.	5.9	4
46	Two-Dimensional Protective Layers of MX₃ to Stabilize Lithium and Sodium Metal Anodes. ACS Applied Energy Materials, 2021, 4, 8653-8659.	5.1	4
47	Light-controlled convergence of photogenerated carriers and reactants to boost photocatalytic performance. Journal of Catalysis, 2021, 400, 1-9.	6.2	4
48	Correlation-driven Lifshitz transition in electron-doped iron selenides (Li,Fe)OHFeSe. Physical Review B, 2018, 98, .	3.2	3
49	First-Principle Prediction on STM Tip Manipulation of Ti Adatom on Two-Dimensional Monolayer YBr3. Scanning, 2019, 2019, 1-7.	1.5	3
50	Crystallization of High Silica RHO Zeolite with Self-Assembled Cs⁺-18-crown-6 Sandwich Complex. Crystal Growth and Design, 2019, 19, 3389-3396.	3.0	3
51	Probing Quantum Capacitance of Typical Two-Dimensional Lattices Based on the Tight-Binding Model. Journal of Physical Chemistry C, 2022, 126, 1256-1263.	3.1	3
52	Charge and spin orderings in triangular<i>t</i>â€“<i>J</i>â€“<i>V</i>model with quarter filling: application to Na_{0.5}CoO₂. Journal of Physics Condensed Matter, 2009, 21, 205602.	1.8	2
53	Phase separation of model on a triangular lattice: Possible application to heavily doped NaxCoO2. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 4718-4723.	2.1	2
54	Magnetoresistance Crossover in Cobalt/Poly(3-hexylthiophene,2,5-diyl) Hybrid Films Due to the Interface Effect. Physical Review Applied, 2019, 11, .	3.8	2

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55	Design and In Situ Growth of Cu ₂ Oâ€Blended Heterojunction Directed by Energyâ€Band Engineering: Toward High Photoelectrochemical Performance. Advanced Materials Interfaces, 0, , 2101690.	3.7	2
56	Video Content Classification Using Time-Sync Comments and Titles. , 2022, , .		2
57	Tritium diffusion in a Li2TiO3 crystal terminated with the (001) surface from first-principles calculations. Physical Chemistry Chemical Physics, 2020, 22, 27206-27213.	2.8	1
58	Organic Photocathode Supported by Copper Nanosheets Array for Overall Water Splitting. Chemistry - A European Journal, 2021, , e202103495.	3.3	1
59	Innentitelbild: A Semi-Conductive Copper-Organic Framework with Two Types of Photocatalytic Activity (Angew. Chem. 16/2016). Angewandte Chemie, 2016, 128, 4922-4922.	2.0	0
60	Electronic structures and anisotropic carrier mobilities of monolayer ternary metal iodides MLaI₅ (M=Mg, Ca, Sr, Ba). Journal of Physics Condensed Matter, 2021, 33, 355301.	1.8	0