Wei-Hua Wang

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	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
3	Molecular dynamics simulations of the initial oxidation process on ferritic Fe–Cr alloy surfaces. RSC Advances, 2022, 12, 9501-9511.	3.6	5
4	Titanium Nitride Protected Cuprous Oxide Photocathode for Stable and Efficient Water Reduction. ACS Applied Energy Materials, 2022, 5, 770-776.	5.1	6
5	Video Content Classification Using Time-Sync Comments and Titles. , 2022, , .		2
6	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
7	Electronic structures and anisotropic carrier mobilities of monolayer ternary metal iodides MLal ₅ (M=Mg, Ca, Sr, Ba). Journal of Physics Condensed Matter, 2021, 33, 355301.	1.8	0
8	Ferroelectricâ€Like Behavior in TaN/Highâ€k/Si System Based on Amorphous Oxide. Advanced Electronic Materials, 2021, 7, 2100414.	5.1	12
9	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
10	Two-Dimensional Protective Layers of MX ₃ to Stabilize Lithium and Sodium Metal Anodes. ACS Applied Energy Materials, 2021, 4, 8653-8659.	5.1	4
11	Light-controlled convergence of photogenerated carriers and reactants to boost photocatalytic performance. Journal of Catalysis, 2021, 400, 1-9.	6.2	4
12	Dehydration of Electrochemically Protonated Oxide: SrCoO ₂ with Square Spin Tubes. Journal of the American Chemical Society, 2021, 143, 17517-17525.	13.7	15
13	Organic Photocathode Supported by Copper Nanosheets Array for Overall Water Splitting. Chemistry - A European Journal, 2021, , e202103495.	3.3	1
14	ITO regulated high-performance n-Si/ITO/α-Fe2O3 Z-scheme heterostructure towards photoelectrochemical water splitting. Journal of Catalysis, 2020, 381, 501-507.	6.2	20
15	Metallic Monolayer Ta ₂ CS ₂ : An Anode Candidate for Li ⁺ , Na ⁺ , K ⁺ , and Ca ²⁺ Ion Batteries. ACS Applied Energy Materials, 2020, 3, 10695-10701.	5.1	23
16	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
17	Ideal two-dimensional solid electrolytes for fast ion transport: metal trihalides MX3 with intrinsic atomic pores. Nanoscale, 2020, 12, 7188-7195.	5.6	9
18	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

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19	First-Principle Prediction on STM Tip Manipulation of Ti Adatom on Two-Dimensional Monolayer YBr3. Scanning, 2019, 2019, 1-7.	1.5	3
20	Molecularly Thin Electrolyte for All Solid-State Nonvolatile Two-Dimensional Crystal Memory. Nano Letters, 2019, 19, 8911-8919.	9.1	6
21	Origin of theoretical pseudocapacitance of two-dimensional supercapacitor electrodes Ti ₃ C ₂ T ₂ (T = bare, O, S). Journal of Materials Chemistry A, 2019, 7, 16231-16238.	10.3	26
22	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
23	Magnetic borophenes from an evolutionary search. Physical Review B, 2019, 99, .	3.2	25
24	Improved carrier doping strategy of monolayer MoS2 through two-dimensional solid electrolyte of YBr3. Applied Physics Letters, 2019, 114, .	3.3	9
25	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
26	Exploring the microscopic mechanism of pseudocapacitance with electronic structures in monolayer 1T-MoS ₂ electrodes for supercapacitors. Materials Chemistry Frontiers, 2019, 3, 1310-1316.	5.9	4
27	TiO ₂ –P3HT:PCBM photoelectrochemical tandem cells for solar-driven overall water splitting. Journal of Materials Chemistry A, 2018, 6, 4032-4039.	10.3	28
28	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
29	First Principles Study of Tritium Diffusion in Li2TiO3 Crystal with Lithium Vacancy. Materials, 2018, 11, 2383.	2.9	16
30	Correlation-driven Lifshitz transition in electron-doped iron selenides (Li,Fe)OHFeSe. Physical Review B, 2018, 98, .	3.2	3
31	Zinc-Blende CdS Nanocubes with Coordinated Facets for Photocatalytic Water Splitting. ACS Catalysis, 2017, 7, 1470-1477.	11.2	83
32	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
33	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
34	Schottky Barrier Height of Pd/MoS ₂ Contact by Large Area Photoemission Spectroscopy. ACS Applied Materials & Interfaces, 2017, 9, 38977-38983.	8.0	36
35	Electronic structures and band alignments of monolayer metal trihalide semiconductors MX ₃ . Journal of Materials Chemistry C, 2017, 5, 9066-9071.	5.5	45
36	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

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37	A Spatially Separated Organic–Inorganic Hybrid Photoelectrochemical Cell for Unassisted Overall Water Splitting. ACS Catalysis, 2017, 7, 5308-5315.	11.2	33
38	Electric-field control of ferromagnetism through oxygen ion gating. Nature Communications, 2017, 8, 2156.	12.8	85
39	A Semiâ€Conductive Copper–Organic Framework with Two Types of Photocatalytic Activity. Angewandte Chemie - International Edition, 2016, 55, 4938-4942.	13.8	164
40	A Semi onductive Copper–Organic Framework with Two Types of Photocatalytic Activity. Angewandte Chemie, 2016, 128, 5022-5026.	2.0	19
41	Elucidating dz2 orbital selective catalytic activity in brownmillerite Ca2Mn2O5. AlP Advances, 2016, 6, 095210.	1.3	6
42	A class of monolayer metal halogenides MX2: Electronic structures and band alignments. Applied Physics Letters, 2016, 108, .	3.3	49
43	Electronic properties and native point defects of high efficient NO oxidation catalysts SmMn2O5. Applied Physics Letters, 2016, 109, .	3.3	27
44	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
45	Efficient photo-degradation of dyes using CuWO ₄ nanoparticles with electron sacrificial agents: a combination of experimental and theoretical exploration. RSC Advances, 2016, 6, 953-959.	3.6	29
46	Origin of Indium Diffusion in High- <i>k</i> Oxide HfO ₂ . ACS Applied Materials & Interfaces, 2016, 8, 7595-7600.	8.0	28
47	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
48	Identifying the descriptor governing NO oxidation on mullite Sm(Y, Tb, Gd,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 2016, 6, 3971-3975.	307 Td (I 4.1	_u)Mn _{2 44}
49	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
50	Ab initio study of doping effects on LiMnO ₂ and Li ₂ MnO ₃ cathode materials for Li-ion batteries. Journal of Materials Chemistry A, 2015, 3, 8489-8500.	10.3	102
51	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
52	Synergistic synthesis of quasi-monocrystal CdS nanoboxes with high-energy facets. Journal of Materials Chemistry A, 2015, 3, 23106-23112.	10.3	5
53	Band alignment of two-dimensional transition metal dichalcogenides: Application in tunnel field effect transistors. Applied Physics Letters, 2013, 103, .	3.3	657
54	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:mrow </mml:msub>S<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:mrow </mml:msub>. Physical Review B, 2013, 87, .</mml:math </mml:math 	3.2	6

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55	Room-temperature ferromagnetism in nanocrystalline Cu/Cu2O core-shell structures prepared by magnetron sputtering. APL Materials, 2013, 1, .	5.1	15
56	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
57	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
58	Charge and spin orderings in triangular <i>t</i> – <i>J</i> – <i>V</i> model with quarter filling: application to Na _{0.5} CoO ₂ . Journal of Physics Condensed Matter, 2009, 21, 205602.	1.8	2
59	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
60	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