Haiying He

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	MoO _{<i>x</i>} S _{<i>y</i>} /Ni ₃ S ₂ Microspheres on Ni Foam as Highly Efficient, Durable Electrocatalysts for Hydrogen Evolution Reaction. Chemistry of Materials, 2022, 34, 798-808.	6.7	26
2	Designing silicon carbide heterostructures for quantum information science: challenges and opportunities. Materials for Quantum Technology, 2022, 2, 023001.	3.1	6
3	Dynamically Stable Active Sites from Surface Evolution of Perovskite Materials during the Oxygen Evolution Reaction. Journal of the American Chemical Society, 2021, 143, 2741-2750.	13.7	156
4	First-principles study of the electronic, magnetic and optical properties of Fe3Se4 in its monoclinic phase. Journal of Magnetism and Magnetic Materials, 2020, 498, 166157.	2.3	6
5	Highly selective electrocatalytic CO2 reduction to ethanol by metallic clusters dynamically formed from atomically dispersed copper. Nature Energy, 2020, 5, 623-632.	39.5	393
6	Modulating reactivity and stability of metallic lithium <i>via</i> atomic doping. Journal of Materials Chemistry A, 2020, 8, 10363-10369.	10.3	18
7	Dynamic stability of active sites in hydr(oxy)oxides for the oxygen evolution reaction. Nature Energy, 2020, 5, 222-230.	39.5	540
8	On-device lead sequestration for perovskite solar cells. Nature, 2020, 578, 555-558.	27.8	284
9	Hierarchical Nanoassembly of MoS ₂ /Co ₉ S ₈ /Ni ₃ S ₂ /Ni as a Highly Efficient Electrocatalyst for Overall Water Splitting in a Wide pH Range. Journal of the American Chemical Society. 2019, 141, 10417-10430.	13.7	653
10	Silicene-supported TiO2 nanostructures: a theoretical study of electronic and optical properties. Physical Chemistry Chemical Physics, 2019, 21, 9335-9341.	2.8	6
11	Silicene catalyzed reduction of nitrobenzene to aniline: A mechanistic study. Chemical Physics Letters, 2018, 695, 228-234.	2.6	13
12	Interaction of silicene with amino acid analogues—from physical to chemical adsorption in gas and solvated phases. 2D Materials, 2018, 5, 015012.	4.4	8
13	Graphene-Supported Monometallic and Bimetallic Dimers for Electrochemical CO2 Reduction. Journal of Physical Chemistry C, 2018, 122, 28629-28636.	3.1	27
14	Electrochemical reduction of CO ₂ on graphene supported transition metals – towards single atom catalysts. Physical Chemistry Chemical Physics, 2017, 19, 11436-11446.	2.8	86
15	Spin-dependent electron transport in C and Ge doped BN monolayers. Physical Chemistry Chemical Physics, 2017, 19, 30370-30380.	2.8	7
16	Single-Electron Activation of CO ₂ on Graphene-Supported ZnO Nanoclusters: Effects of Doping in the Support. Journal of Physical Chemistry C, 2016, 120, 16732-16740.	3.1	14
17	Interaction of metallic clusters with biologically active curcumin molecules. Chemical Physics Letters, 2015, 636, 163-166.	2.6	0
18	Surface-dependence of interfacial binding strength between zinc oxide and graphene. RSC Advances, 2015, 5, 65719-65724.	3.6	15

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19	Pressure and electric field-induced metallization in the phase-engineered ZrX ₂ (X = S, Se,) Tj ETQq1	1 0,784314 2.8	4 rgBT /Over
20	Nature of Interaction between Semiconducting Nanostructures and Biomolecules: Chalcogenide QDs and BNNT with DNA Molecules. Journal of Physical Chemistry C, 2015, 119, 25965-25973.	3.1	27
21	Decoding the mechanism of the mechanical transfer of a GaN-based heterostructure via an h-BN release layer in a device configuration. Applied Physics Letters, 2014, 105, 121605.	3.3	11
22	Effect of Si doping on the electronic properties of BN monolayer. Nanoscale, 2014, 6, 5526-5531.	5.6	42
23	Computational studies of electrochemical CO ₂ reduction on subnanometer transition metal clusters. Physical Chemistry Chemical Physics, 2014, 16, 26584-26599.	2.8	62
24	Studies on phase stability, mechanical, optical and electronic properties of a new Gd2CaZnO5 phosphor system for LEDs. CrystEngComm, 2014, 16, 1652.	2.6	10
25	On the variation of dissolution rates at the orthoclase (0 0 1) surface with pH and temperature. Geochimica Et Cosmochimica Acta, 2014, 141, 598-611.	3.9	16
26	A theoretical study of structural and electronic properties of alkaline-earth fluoride clusters. Computational and Theoretical Chemistry, 2014, 1043, 24-30.	2.5	12
27	Stacking and electric field effects in atomically thin layers of GaN. Journal of Physics Condensed Matter, 2013, 25, 345302.	1.8	68
28	Surface dealloyed PtCo nanoparticles supported on carbon nanotube: facile synthesis and promising application for anion exchange membrane direct crude glycerol fuel cell. Green Chemistry, 2013, 15, 1133.	9.0	71
29	Electron tunneling characteristics of a cubic quantum dot, (PbS)32. Journal of Chemical Physics, 2013, 139, 244307.	3.0	13
30	Firstâ€Principles Study of Hydrolysis Reaction Barriers in a Sodium Borosilicate Glass. International Journal of Applied Glass Science, 2013, 4, 395-407.	2.0	66
31	Conformation vs voltage gating in a molecular transistor: A first-principles quantum chemical study. , 2012, , .		0
32	Photoredox Reactions and the Catalytic Cycle for Carbon Dioxide Fixation and Methanogenesis on Metal Oxides. Journal of Physical Chemistry C, 2012, 116, 9450-9460.	3.1	129
33	Heteroatom-Transfer Coupled Photoreduction and Carbon Dioxide Fixation on Metal Oxides. Journal of Physical Chemistry C, 2012, 116, 9461-9471.	3.1	45
34	Computational screening of dopants for photocatalytic two-electron reduction of CO2 on anatase (101) surfaces. Energy and Environmental Science, 2012, 5, 6196.	30.8	138
35	Role of Water and Carbonates in Photocatalytic Transformation of CO ₂ to CH ₄ on Titania. Journal of the American Chemical Society, 2011, 133, 3964-3971.	13.7	416
36	Metal-like Electrical Conductance in Boron Fullerenes. Journal of Physical Chemistry C, 2010, 114, 4149-4152.	3.1	30

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37	A Theoretical Study of CO ₂ Anions on Anatase (101) Surface. Journal of Physical Chemistry C, 2010, 114, 21474-21481.	3.1	159
38	Lengthâ€dependence of electron transfer coupling matrix in polyene wires: Ab initio molecular orbital theory study. International Journal of Quantum Chemistry, 2009, 109, 1302-1310.	2.0	3
39	Asymmetric Currents in a Donorâ d'Bridgeâ d'Acceptor Single Molecule: Revisit of the Aviramâ d'Ratner Diode. Journal of Physical Chemistry C, 2009, 113, 1575-1579.	3.1	30
40	Highly efficient (Cs8V) superatom-based spin-polarizer. Applied Physics Letters, 2009, 95, .	3.3	26
41	Electronic conduction in a model three-terminal molecular transistor. Nanotechnology, 2008, 19, 505203.	2.6	16
42	Functionalized Nanopore-Embedded Electrodes for Rapid DNA Sequencing. Journal of Physical Chemistry C, 2008, 112, 3456-3459.	3.1	73
43	Interaction of Metallic Nanoparticles with a Biologically Active Molecule, Dopamine. Journal of Physical Chemistry B, 2008, 112, 15256-15259.	2.6	22
44	Interaction of nanomaterials with biological molecules: Manganese and dopamine. , 2008, , .		0
45	Electron Transport in Boron Fullerenes. , 2008, , .		2
46	Mechanism of Electrical Rectification in a Unimolecular Donor-Bridge (Ï \in)-Acceptor Diode. , 2007, , .		0
47	Electronic structure mechanism of spin-polarized electron transport in a Ni–C60–Ni system. Chemical Physics Letters, 2007, 439, 110-114.	2.6	15
48	Spin-Polarized Electron Transport via a C <inf>60</inf> Molecule. , 2006, , .		0
49	Geometry, electronic properties, and thermodynamics of pure and Al-doped Li clusters. Physical Review B, 2006, 74, .	3.2	15
50	First-principles study of the structural, electronic, and optical properties ofGa2O3in its monoclinic and hexagonal phases. Physical Review B, 2006, 74, .	3.2	510
51	Theoretical study of molecule mediated spin-polarized electron tunneling between magnetic materials. Chemical Physics Letters, 2006, 428, 411-415.	2.6	4
52	Spin-polarized electron transport of a self-assembled organic monolayer on a Ni(111) substrate: An organic spin switch. Physical Review B, 2006, 73, .	3.2	35
53	Electronic and thermodynamic properties of β-Ga2O3. Applied Physics Letters, 2006, 88, 261904.	3.3	125
54	Molecular modeling of water diffusion in amorphous SiC. Journal of Applied Physics, 2005, 98, 023519.	2.5	3

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55	Structure and magnetic properties of cobalt nanoplatelets. Materials Letters, 2004, 58, 2506-2509.	2.6	22
56	Weak ferromagnetism in Re0.67Ca0.33FeO3 (Re=La, Sm, Gd) nanoparticles. Journal of Magnetism and Magnetic Materials, 2003, 263, 154-160.	2.3	1
57	Structures and magnetic properties of Nd1â^'xCaxFeO3 nanoparticles. Journal of Applied Physics, 2002, 92, 7504-7509.	2.5	12
58	Microstructure and Magnetic Properties of La1?xSrxFeO3 Nanoparticles. Physica Status Solidi A, 2002, 191, 255-259.	1.7	22
59	Crystal structure, electronic structure, and magnetic properties of bismuth-strontium ferrites. Journal of Alloys and Compounds, 2001, 315, 259-264.	5.5	115
60	Spin-dependent electron transport along a molecular wire in a metal (probe)-vacuum-molecule-metal system: the effect of the size and the shape of the probe tip. , 0, , .		1
61	Spin-Polarized Electron Transport via a C>inf<60>/inf <molecule. ,="" .<="" 0,="" td=""><td></td><td>0</td></molecule.>		0
62	Electron transport properties of PAI12-based cluster complexes. Nanoscale Advances, 0, , .	4.6	1