

# Haiying He

## List of Publications by Year in descending order

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62  
papers

4,675  
citations

218677

26  
h-index

161849

54  
g-index

63  
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63  
docs citations

63  
times ranked

6821  
citing authors

#	ARTICLE	IF	CITATIONS
1	Hierarchical Nanoassembly of MoS <sub>2</sub> /Co <sub>9</sub> S <sub>8</sub> /Ni <sub>3</sub> S <sub>2</sub> /Ni as a Highly Efficient Electrocatalyst for Overall Water Splitting in a Wide pH Range. <i>Journal of the American Chemical Society</i> , 2019, 141, 10417-10430.	13.7	653
2	Dynamic stability of active sites in hydr(oxy)oxides for the oxygen evolution reaction. <i>Nature Energy</i> , 2020, 5, 222-230.	39.5	540
3	First-principles study of the structural, electronic, and optical properties of Ga <sub>2</sub> O <sub>3</sub> in its monoclinic and hexagonal phases. <i>Physical Review B</i> , 2006, 74, .	3.2	510
4	Role of Water and Carbonates in Photocatalytic Transformation of CO <sub>2</sub> to CH <sub>4</sub> on Titania. <i>Journal of the American Chemical Society</i> , 2011, 133, 3964-3971.	13.7	416
5	Highly selective electrocatalytic CO <sub>2</sub> reduction to ethanol by metallic clusters dynamically formed from atomically dispersed copper. <i>Nature Energy</i> , 2020, 5, 623-632.	39.5	393
6	On-device lead sequestration for perovskite solar cells. <i>Nature</i> , 2020, 578, 555-558.	27.8	284
7	A Theoretical Study of CO <sub>2</sub> Anions on Anatase (101) Surface. <i>Journal of Physical Chemistry C</i> , 2010, 114, 21474-21481.	3.1	159
8	Dynamically Stable Active Sites from Surface Evolution of Perovskite Materials during the Oxygen Evolution Reaction. <i>Journal of the American Chemical Society</i> , 2021, 143, 2741-2750.	13.7	156
9	Computational screening of dopants for photocatalytic two-electron reduction of CO <sub>2</sub> on anatase (101) surfaces. <i>Energy and Environmental Science</i> , 2012, 5, 6196.	30.8	138
10	Photoredox Reactions and the Catalytic Cycle for Carbon Dioxide Fixation and Methanogenesis on Metal Oxides. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9450-9460.	3.1	129
11	Electronic and thermodynamic properties of Î²-Ga <sub>2</sub> O <sub>3</sub> . <i>Applied Physics Letters</i> , 2006, 88, 261904.	3.3	125
12	Crystal structure, electronic structure, and magnetic properties of bismuth-strontium ferrites. <i>Journal of Alloys and Compounds</i> , 2001, 315, 259-264.	5.5	115
13	Electrochemical reduction of CO <sub>2</sub> on graphene supported transition metals “towards single atom catalysts. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 11436-11446.	2.8	86
14	Functionalized Nanopore-Embedded Electrodes for Rapid DNA Sequencing. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3456-3459.	3.1	73
15	Surface dealloyed PtCo nanoparticles supported on carbon nanotube: facile synthesis and promising application for anion exchange membrane direct crude glycerol fuel cell. <i>Green Chemistry</i> , 2013, 15, 1133.	9.0	71
16	Stacking and electric field effects in atomically thin layers of GaN. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 345302.	1.8	68
17	First-Principles Study of Hydrolysis Reaction Barriers in a Sodium Borosilicate Glass. <i>International Journal of Applied Glass Science</i> , 2013, 4, 395-407.	2.0	66
18	Computational studies of electrochemical CO <sub>2</sub> reduction on subnanometer transition metal clusters. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 26584-26599.	2.8	62

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19	Heteroatom-Transfer Coupled Photoreduction and Carbon Dioxide Fixation on Metal Oxides. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9461-9471.	3.1	45
20	Effect of Si doping on the electronic properties of BN monolayer. <i>Nanoscale</i> , 2014, 6, 5526-5531.	5.6	42
21	Pressure and electric field-induced metallization in the phase-engineered $ZrX_2$ ( $X = S, Se$ ). <i>Tj ETQq1 1 0,784314 rgBT /Over</i>	2.8	36
22	Spin-polarized electron transport of a self-assembled organic monolayer on a Ni(111) substrate: An organic spin switch. <i>Physical Review B</i> , 2006, 73, .	3.2	35
23	Asymmetric Currents in a Donor-Bridge-Acceptor Single Molecule: Revisit of the Aviram-Ratner Diode. <i>Journal of Physical Chemistry C</i> , 2009, 113, 1575-1579.	3.1	30
24	Metal-like Electrical Conductance in Boron Fullerenes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 4149-4152.	3.1	30
25	Nature of Interaction between Semiconducting Nanostructures and Biomolecules: Chalcogenide QDs and BNNT with DNA Molecules. <i>Journal of Physical Chemistry C</i> , 2015, 119, 25965-25973.	3.1	27
26	Graphene-Supported Monometallic and Bimetallic Dimers for Electrochemical CO <sub>2</sub> Reduction. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28629-28636.	3.1	27
27	Highly efficient (Cs <sub>8</sub> V) superatom-based spin-polarizer. <i>Applied Physics Letters</i> , 2009, 95, .	3.3	26
28	MoO <sub>x</sub> S <sub>y</sub> /Ni <sub>3</sub> S <sub>2</sub> Microspheres on Ni Foam as Highly Efficient, Durable Electrocatalysts for Hydrogen Evolution Reaction. <i>Chemistry of Materials</i> , 2022, 34, 798-808.	6.7	26
29	Microstructure and Magnetic Properties of La <sub>1-x</sub> Sr <sub>x</sub> FeO <sub>3</sub> Nanoparticles. <i>Physica Status Solidi A</i> , 2002, 191, 255-259.	1.7	22
30	Structure and magnetic properties of cobalt nanoplatelets. <i>Materials Letters</i> , 2004, 58, 2506-2509.	2.6	22
31	Interaction of Metallic Nanoparticles with a Biologically Active Molecule, Dopamine. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15256-15259.	2.6	22
32	Modulating reactivity and stability of metallic lithium via atomic doping. <i>Journal of Materials Chemistry A</i> , 2020, 8, 10363-10369.	10.3	18
33	Electronic conduction in a model three-terminal molecular transistor. <i>Nanotechnology</i> , 2008, 19, 505203.	2.6	16
34	On the variation of dissolution rates at the orthoclase (0 0 1) surface with pH and temperature. <i>Geochimica Et Cosmochimica Acta</i> , 2014, 141, 598-611.	3.9	16
35	Geometry, electronic properties, and thermodynamics of pure and Al-doped Li clusters. <i>Physical Review B</i> , 2006, 74, .	3.2	15
36	Electronic structure mechanism of spin-polarized electron transport in a Ni@C <sub>60</sub> @Ni system. <i>Chemical Physics Letters</i> , 2007, 439, 110-114.	2.6	15

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37	Surface-dependence of interfacial binding strength between zinc oxide and graphene. RSC Advances, 2015, 5, 65719-65724.	3.6	15
38	Single-Electron Activation of CO <sub>2</sub> on Graphene-Supported ZnO Nanoclusters: Effects of Doping in the Support. Journal of Physical Chemistry C, 2016, 120, 16732-16740.	3.1	14
39	Electron tunneling characteristics of a cubic quantum dot, (PbS) <sub>32</sub> . Journal of Chemical Physics, 2013, 139, 244307.	3.0	13
40	Silicene catalyzed reduction of nitrobenzene to aniline: A mechanistic study. Chemical Physics Letters, 2018, 695, 228-234.	2.6	13
41	Structures and magnetic properties of Nd <sub>1-x</sub> Ca <sub>x</sub> FeO <sub>3</sub> nanoparticles. Journal of Applied Physics, 2002, 92, 7504-7509.	2.5	12
42	A theoretical study of structural and electronic properties of alkaline-earth fluoride clusters. Computational and Theoretical Chemistry, 2014, 1043, 24-30.	2.5	12
43	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
44	Studies on phase stability, mechanical, optical and electronic properties of a new Gd <sub>2</sub> CaZnO <sub>5</sub> phosphor system for LEDs. CrystEngComm, 2014, 16, 1652.	2.6	10
45	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
46	Spin-dependent electron transport in C and Ge doped BN monolayers. Physical Chemistry Chemical Physics, 2017, 19, 30370-30380.	2.8	7
47	Silicene-supported TiO <sub>2</sub> nanostructures: a theoretical study of electronic and optical properties. Physical Chemistry Chemical Physics, 2019, 21, 9335-9341.	2.8	6
48	First-principles study of the electronic, magnetic and optical properties of Fe <sub>3</sub> Se <sub>4</sub> in its monoclinic phase. Journal of Magnetism and Magnetic Materials, 2020, 498, 166157.	2.3	6
49	Designing silicon carbide heterostructures for quantum information science: challenges and opportunities. Materials for Quantum Technology, 2022, 2, 023001.	3.1	6
50	Theoretical study of molecule mediated spin-polarized electron tunneling between magnetic materials. Chemical Physics Letters, 2006, 428, 411-415.	2.6	4
51	Molecular modeling of water diffusion in amorphous SiC. Journal of Applied Physics, 2005, 98, 023519.	2.5	3
52	Length-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
53	Electron Transport in Boron Fullerenes. , 2008, , .		2
54	Weak ferromagnetism in Re <sub>0.67</sub> Ca <sub>0.33</sub> FeO <sub>3</sub> (Re=La, Sm, Gd) nanoparticles. Journal of Magnetism and Magnetic Materials, 2003, 263, 154-160.	2.3	1

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55	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
56	Electron transport properties of PA12-based cluster complexes. Nanoscale Advances, 0, , .	4.6	1
57	Spin-Polarized Electron Transport via a C<inf>60</inf>Molecule. , 2006, , .		0
58	Spin-Polarized Electron Transport via a C>inf<60>/inf<Molecule. , 0, , .		0
59	Mechanism of Electrical Rectification in a Unimolecular Donor-Bridge (i€)-Acceptor Diode. , 2007, , .		0
60	Interaction of nanomaterials with biological molecules: Manganese and dopamine. , 2008, , .		0
61	Conformation vs voltage gating in a molecular transistor: A first-principles quantum chemical study. , 2012, , .		0
62	Interaction of metallic clusters with biologically active curcumin molecules. Chemical Physics Letters, 2015, 636, 163-166.	2.6	0