

# Gang Zhou

## List of Publications by Year in descending order

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57  
papers

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citations

201674  
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138484  
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59  
docs citations

59  
times ranked

8669  
citing authors

#	ARTICLE	IF	CITATIONS
1	Identification of active sites available for hydrogen evolution of Single-Atom Ni1/TiO2 catalysts. Applied Surface Science, 2022, 579, 152139.	6.1	11
2	Insight into enhanced hydrogen evolution of single-atom Cu1/TiO2 catalysts from first principles. International Journal of Hydrogen Energy, 2022, 47, 4653-4661.	7.1	15
3	Hydrogen evolution/spillover effect of single cobalt atom on anatase TiO2 from first-principles calculations. Applied Surface Science, 2021, 536, 147831.	6.1	13
4	Engineering the Atomic Interface with Single Platinum Atoms for Enhanced Photocatalytic Hydrogen Production. Angewandte Chemie, 2020, 132, 1311-1317.	2.0	59
5	Engineering the Atomic Interface with Single Platinum Atoms for Enhanced Photocatalytic Hydrogen Production. Angewandte Chemie - International Edition, 2020, 59, 1295-1301.	13.8	344
6	Effects of a graphene substrate on the structure and properties of atomically thin metal sheets. Physical Chemistry Chemical Physics, 2020, 22, 667-673.	2.8	6
7	Lattice-Strain Control of Flexible Janus Indium Chalcogenide Monolayers for Photocatalytic Water Splitting. Journal of Physical Chemistry C, 2020, 124, 167-174.	3.1	30
8	2D van der Waals heterostructures of graphitic BCN as direct Z-scheme photocatalysts for overall water splitting: the role of polar $\pi$ -conjugated moieties. Physical Chemistry Chemical Physics, 2020, 22, 23735-23742.	2.8	16
9	N-Promoted Ru <sub>1</sub> /TiO <sub>2</sub> single-atom catalysts for photocatalytic water splitting for hydrogen production: a density functional theory study. Physical Chemistry Chemical Physics, 2020, 22, 11392-11399.	2.8	28
10	Metal/graphene heterobilayers as hydrogen evolution reaction cathodes: a first-principles study. Physical Chemistry Chemical Physics, 2019, 21, 4594-4599.	2.8	6
11	Surface Oxidation of AuNi Heterodimers to Achieve High Activities toward Hydrogen/Oxygen Evolution and Oxygen Reduction Reactions. Small, 2018, 14, e1703749.	10.0	60
12	A theoretical study on the mechanism of hydrogen evolution on non-precious partially oxidized nickel-based heterostructures for fuel cells. Physical Chemistry Chemical Physics, 2018, 20, 7968-7973.	2.8	15
13	Theoretical investigations of transport properties of organic solvents in cation-functionalized graphene oxide membranes: Implications for drug delivery. Nano Research, 2018, 11, 254-263.	10.4	7
14	Molecule Channels Directed by Cation-Decorated Graphene Oxide Nanosheets and Their Application as Membrane Reactors. Advanced Materials, 2017, 29, 1606093.	21.0	83
15	Theoretical study on in situ synthesis of Pt/Ni Al hydroxide composites by etching of Pt Ni nanoparticles. Chemical Physics Letters, 2017, 679, 200-206.	2.6	3
16	Conditions for magnetic and electronic properties of ultrathin Ni-Fe hydroxide nanosheets as catalysts: a DFT+U study. Science China Materials, 2017, 60, 664-673.	6.3	7
17	Design of ultrathin Pt-Mo-Ni nanowire catalysts for ethanol electrooxidation. Science Advances, 2017, 3, e1603068.	10.3	224
18	Modulating fcc and hcp Ruthenium on the Surface of Palladium-Copper Alloy through Tunable Lattice Mismatch. Angewandte Chemie, 2016, 128, 5591-5595.	2.0	33

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19	Intermetallic Ni <sub>x</sub> M <sub>y</sub> ( <i>M</i> = Ga and Sn) Nanocrystals: A Nonprecious Metal Catalyst for Semihydrogenation of Alkynes. <i>Advanced Materials</i> , 2016, 28, 4747-4754.	21.0	145
20	Modulating fcc and hcp Ruthenium on the Surface of Palladium-Copper Alloy through Tunable Lattice Mismatch. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 5501-5505.	13.8	95
21	Availability of surface boron species in improved oxygen reduction activity of Pt catalysts: A first-principles study. <i>Journal of Chemical Physics</i> , 2016, 144, 144706.	3.0	7
22	Single Cobalt Atoms with Precise N-Coordination as Superior Oxygen Reduction Reaction Catalysts. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 10800-10805.	13.8	1,836
23	Single Cobalt Atoms with Precise N-Coordination as Superior Oxygen Reduction Reaction Catalysts. <i>Angewandte Chemie</i> , 2016, 128, 10958-10963.	2.0	373
24	Amorphous nickel boride membrane on a platinum-nickel alloy surface for enhanced oxygen reduction reaction. <i>Nature Communications</i> , 2016, 7, 12362.	12.8	190
25	Synergetic Integration of Cu <sub>1.94</sub> S-Zn <sub>x</sub> Cd <sub>1-x</sub> Heteronanorods for Enhanced Visible-Light-Driven Photocatalytic Hydrogen Production. <i>Journal of the American Chemical Society</i> , 2016, 138, 4286-4289.	13.7	257
26	Utilization of Active Ni to Fabricate Pt-Ni Nanoframe/NiAl Layered Double Hydroxide Multifunctional Catalyst through In Situ Precipitation. <i>Chemistry - A European Journal</i> , 2015, 21, 13181-13185.	3.3	19
27	Rational synthesis and the structure-property relationships of nanoheterostructures: a combinative study of experiments and theory. <i>NPG Asia Materials</i> , 2015, 7, e164-e164.	7.9	20
28	Colloidal 2D Lateral Nanoheterostructures: A Case Study of Site-Selective Growth of CdS Nanodots onto Bi <sub>2</sub> Se <sub>3</sub> Nanosheets. <i>Nano Letters</i> , 2015, 15, 4200-4205.	9.1	17
29	First principles study of ruthenium( <i>ii</i> ) sensitizer adsorption on anatase TiO <sub>2</sub> (001) surface. <i>RSC Advances</i> , 2015, 5, 60230-60236.	3.6	7
30	Strong metal-support interaction in size-controlled monodisperse palladium-hematite nano-heterostructures during a liquid-solid heterogeneous catalysis. <i>Science China Materials</i> , 2014, 57, 34-41.	6.3	19
31	A 1D/2D Helical CdS/ZnIn <sub>2</sub> S <sub>4</sub> Nano-Heterostructure. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 2339-2343.	13.8	232
32	Ferromagnetism and topological surface states of manganese doped Bi <sub>2</sub> Te <sub>3</sub> : Insights from density-functional calculations. <i>Journal of Chemical Physics</i> , 2014, 140, 124704.	3.0	19
33	Ultrathin rhodium nanosheets. <i>Nature Communications</i> , 2014, 5, 3093.	12.8	428
34	Antisite Atom Segregation in Porous Boron Nitride Nanotubes: Formation Mechanism and Characterization. <i>Journal of Physical Chemistry C</i> , 2012, 116, 22051-22056.	3.1	2
35	Phonon thermal conductivity of GaN nanotubes. <i>Journal of Applied Physics</i> , 2012, 112, .	2.5	14
36	Formation, Morphology, and Effect of Complex Defects in Boron Nitride Nanotubes: An ab initio Calculation. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12782-12788.	3.1	7

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37	Ab initio Study of Half-Metallicity and Magnetism of Complex Organometallic Molecular Wires. Journal of Physical Chemistry C, 2011, 115, 7292-7297.	3.1	19
38	Trends in charge transfer and spin alignment of metallocene on graphene. Physical Review B, 2011, 83, .	3.2	15
39	Theoretical Modeling and Computational Simulation of Electronic Properties of Nanomaterials. Journal of Nanomaterials, 2011, 2011, 1-2.	2.7	0
40	Optimizing photoelectrochemical properties of $\text{TiO}_2$ chemical codoping. Physical Review B, 2010, 82, .	3.2	62
41	Spontaneous edge-defect formation and defect-induced conductance suppression in graphene nanoribbons. Physical Review B, 2010, 82, .	3.2	41
42	Structural and electronic properties of Ge-Si, Sn-Si, and Pb-Si dimers on Si(001) from density-functional calculations. Physical Review B, 2009, 79, .	3.2	1
43	Preparing spin-polarized scanning tunneling microscope probes on capped carbon nanotubes by Fe doping: A first-principles study. Applied Physics Letters, 2009, 94, 193106.	3.3	4
44	Activated dissociation of $\text{O}_2$ on Pb(111) surfaces by Pb adatoms. Physical Review B, 2009, 80, .	3.2	7
45	Magnetism of C Adatoms on BN Nanostructures: Implications for Functional Nanodevices. Journal of the American Chemical Society, 2009, 131, 1796-1801.	13.7	80
46	Half metallicity along the edge of zigzag boron nitride nanoribbons. Physical Review B, 2008, 78, .	3.2	226
47	Alkali-Metal-Doped B80 as High-Capacity Hydrogen Storage Media. Journal of Physical Chemistry C, 2008, 112, 19268-19271.	3.1	107
48	Room-temperature dissociative hydrogen chemisorption on boron-doped fullerenes. Physical Review B, 2008, 77, .	3.2	19
49	Quantum confinement of crystalline silicon nanotubes with nonuniform wall thickness: Implication to modulation doping. Applied Physics Letters, 2007, 91, 103107.	3.3	12
50	Making a field effect transistor on a single graphene nanoribbon by selective doping. Applied Physics Letters, 2007, 91, 253122.	3.3	152
51	Effects of vacancy-carboxyl pair functionalization on electronic properties of carbon nanotubes. Applied Physics Letters, 2006, 89, 173130.	3.3	42
52	Mechanism of nanoelectronic switch based on telescoping carbon nanotubes. Applied Physics Letters, 2006, 88, 173107.	3.3	42
53	Field Emission in Doped Nanotubes. Journal of Nanoscience and Nanotechnology, 2005, 5, 1421-1434.	0.9	31
54	Long periodic oscillation of electronic properties in capped finite-length armchair carbon nanotubes. Physical Review B, 2005, 71, .	3.2	6

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55	Spontaneous polarizations of ultrashort-period epitaxial $\text{KNbO}_3/\text{(KTaO}_3\text{)}_m$ superlattices: An ab initio investigation. <i>Applied Physics Letters</i> , 2005, 86, 232903.	3.3	19
56	Single electron emission from the closed-tips of single-walled carbon nanotubes. <i>Journal of Chemical Physics</i> , 2004, 121, 12600.	3.0	6
57	Dimensional effects on field emission properties of the body for single-walled carbon nanotube. <i>Applied Physics Letters</i> , 2001, 79, 836-838.	3.3	42