Jijun Zhao

List of Publications by Citations

650 papers	23,162 citations	72 h-index	125 g-index
678 ext. papers	26,673 ext. citations	5.3 avg, IF	7.47 L-index

#	Paper	IF	Citations
650	Gas molecule adsorption in carbon nanotubes and nanotube bundles. *Nanotechnology*, **2002**, 13, 195-200	3.4	979
649	Rise of silicene: A competitive 2D material. *Progress in Materials Science*, **2016**, 83, 24-151	42.2	548
648	Metal-Organic-Framework-Derived Hybrid Carbon Nanocages as a Bifunctional Electrocatalyst for Oxygen Reduction and Evolution. *Advanced Materials*, **2017**, 29, 1700874	24	518
647	Graphene oxide: A promising nanomaterial for energy and environmental applications. *Nano Energy* , **2015**, 16, 488-515	17.1	406
646	Atomic-level insight into super-efficient electrocatalytic oxygen evolution on iron and vanadium co-doped nickel (oxy)hydroxide. *Nature Communications*, **2018**, 9, 2885	17.4	398
645	Density-functional study of Aun(n=2□20) clusters: Lowest-energy structures and electronic properties. *Physical Review B*, **2002**, 66,	3.3	393
644	Facile Ammonia Synthesis from Electrocatalytic N2 Reduction under Ambient Conditions on N-Doped Porous Carbon. *ACS Catalysis*, **2018**, 8, 1186-1191	13.1	392
643	Boosting electrocatalytic oxygen evolution by synergistically coupling layered double hydroxide with MXene. *Nano Energy*, **2018**, 44, 181-190	17.1	304
642	Graphene nucleation on transition metal surface: structure transformation and role of the metal step edge. *Journal of the American Chemical Society*, **2011**, 133, 5009-15	16.4	273
641	First-principles study of Li-intercalated carbon nanotube ropes. *Physical Review Letters*, **2000**, 85, 1706-9	7.4	271
640	Electronic Properties of Carbon Nanotubes with Covalent Sidewall Functionalization. *Journal of Physical Chemistry B*, **2004**, 108, 4227-4230	3.4	252
639	Noncovalent functionalization of carbon nanotubes by aromatic organic molecules. *Applied Physics Letters*, **2003**, 82, 3746-3748	3.4	237
638	Silicene on Substrates: A Way To Preserve or Tune Its Electronic Properties. *Journal of Physical Chemistry C*, **2013**, 117, 10353-10359	3.8	215
637	Structures, mobilities, electronic and magnetic properties of point defects in silicene. *Nanoscale*, **2013**, 5, 9785-92	7.7	202
636	Magnetism of transition-metal/carbon-nanotube hybrid structures. *Physical Review Letters*, **2003**, 90, 257203	7.4	195
635	Mechanical properties of graphene oxides. *Nanoscale*, **2012**, 4, 5910-6	7.7	191
634	Enhanced piezoelectric effect in Janus group-III chalcogenide monolayers. *Applied Physics Letters*, **2017**, 110, 163102	3.4	190

633	Effects of sidewall functionalization on conducting properties of single wall carbon nanotubes. *Nano Letters*, **2006**, 6, 916-9	11.5	185
632	2D covalent triazine framework: a new class of organic photocatalyst for water splitting. *Journal of Materials Chemistry A*, **2015**, 3, 7750-7758	13	183
631	Ultrasensitive Iron-Triggered Nanosized Fe□oOOH Integrated with Graphene for Highly Efficient Oxygen Evolution. *Advanced Energy Materials*, **2017**, 7, 1602148	21.8	177
630	Work functions of pristine and alkali-metal intercalated carbon nanotubes and bundles. *Physical Review B*, **2002**, 65,	3.3	174
629	Novel structures and properties of gold nanowires. *Physical Review Letters*, **2001**, 86, 2046-9	7.4	173
628	Intrinsic strength and failure behaviors of graphene grain boundaries. *ACS Nano*, **2012**, 6, 2704-11	16.7	172
627	Fe-Anchored Graphene Oxide: A Low-Cost and Easily Accessible Catalyst for Low-Temperature CO Oxidation. *Journal of Physical Chemistry C*, **2012**, 116, 2507-2514	3.8	171
626	First-principles calculations of second- and third-order elastic constants for single crystals of arbitrary symmetry. *Physical Review B*, **2007**, 75,	3.3	168
625	Initial geometries, interaction mechanism and high stability of silicene on Ag(111) surface. *Scientific Reports*, **2012**, 2, 861	4.9	167
624	From boron cluster to two-dimensional boron sheet on Cu(111) surface: growth mechanism and hole formation. *Scientific Reports*, **2013**, 3, 3238	4.9	162
623	Heterostructures of MXenes and N-doped graphene as highly active bifunctional electrocatalysts. *Nanoscale*, **2018**, 10, 10876-10883	7.7	154
622	Probing the electronic effect of carbon nanotubes in catalysis: NH(3) synthesis with Ru nanoparticles. *Chemistry - A European Journal*, **2010**, 16, 5379-84	4.8	150
621	Comparative study of hydrogen adsorption on carbon and BN nanotubes. *Journal of Physical Chemistry B*, **2006**, 110, 13363-9	3.4	149
620	Tuning the band gap in silicene by oxidation. *ACS Nano*, **2014**, 8, 10019-25	16.7	147
619	Atomistic insight into the oxidation of monolayer transition metal dichalcogenides: from structures to electronic properties. *RSC Advances*, **2015**, 5, 17572-17581	3.7	144
618	Structural Growth Sequences and Electronic Properties of Zinc Oxide Clusters (ZnO)n (n=2-18). *Journal of Physical Chemistry C*, **2007**, 111, 4956-4963	3.8	141
617	Band Gap Tuning of Hydrogenated Graphene: H Coverage and Configuration Dependence. *Journal of Physical Chemistry C*, **2011**, 115, 3236-3242	3.8	139
616	Structure and electronic properties of Gen (n=2□5) clusters from density-functional theory. *Physical Review B*, **2001**, 64,	3.3	138

615	Correlation between hardness and elastic moduli of the covalent crystals. *Computational Materials Science*, **2011**, 50, 2287-2290	3.2	131
614	B80 and B101-103 clusters: remarkable stability of the core-shell structures established by validated density functionals. *Journal of Chemical Physics*, **2012**, 136, 074302	3.9	131
613	Ultrahigh Rate and Long-Life Sodium-Ion Batteries Enabled by Engineered Surface and Near-Surface Reactions. *Advanced Materials*, **2018**, 30, 1702486	24	130
612	Endohedral silicon fullerenes sinN (27 Journal of the American Chemical Society, **2004**, 126, 13845-9	16.4	125
611	Magic carbon clusters in the chemical vapor deposition growth of graphene. *Journal of the American Chemical Society*, **2012**, 134, 2970-5	16.4	124
610	B(80) and other medium-sized boron clusters: core-shell structures, not hollow cages. *Journal of Physical Chemistry A*, **2010**, 114, 9969-72	2.8	121
609	Structures and electronic properties of Cu20, Ag20, and Au20 clusters with density functional method. *Chemical Physics Letters*, **2003**, 380, 716-720	2.5	121
608	In situ capture of active species and oxidation mechanism of RhB and MB dyes over sunlight-driven Ag/Ag3PO4 plasmonic nanocatalyst. *Applied Catalysis B: Environmental*, **2012**, 125, 538-545	21.8	120
607	Do Composite Single-Walled Nanotubes Have Enhanced Capability for Lithium Storage?. *Chemistry of Materials*, **2005**, 17, 992-1000	9.6	113
606	Quasi-freestanding epitaxial silicene on Ag(111) by oxygen intercalation. *Science Advances*, **2016**, 2, e1600067	14.7	112
605	Hole defects and nitrogen doping in graphene: implication for supercapacitor applications. *ACS Applied Materials & Interfaces*, **2013**, 5, 11184-93	9.5	110
604	Transition metal surface passivation induced graphene edge reconstruction. *Journal of the American Chemical Society*, **2012**, 134, 6204-9	16.4	110
603	Formation of Carbon Clusters in the Initial Stage of Chemical Vapor Deposition Graphene Growth on Ni(111) Surface. *Journal of Physical Chemistry C*, **2011**, 115, 17695-17703	3.8	109
602	Nitrogen-Doped Graphene on Transition Metal Substrates as Efficient Bifunctional Catalysts for Oxygen Reduction and Oxygen Evolution Reactions. *ACS Applied Materials & Interfaces*, **2017**, 9, 22578-22587	9.5	103
601	Graphene oxide as a chemically tunable 2-D material for visible-light photocatalyst applications. *Journal of Catalysis*, **2013**, 299, 204-209	7.3	101
600	Binding energies and electronic structures of adsorbed titanium chains on carbon nanotubes. *Physical Review B*, **2002**, 66,	3.3	100
599	MBene (MnB): a new type of 2D metallic ferromagnet with high Curie temperature. *Nanoscale Horizons*, **2018**, 3, 335-341	10.8	99
598	Appropriate description of intermolecular interactions in the methane hydrates: an assessment of DFT methods. *Journal of Computational Chemistry*, **2013**, 34, 121-31	3.5	99

597	Rapid and energy-efficient microwave pyrolysis for high-yield production of highly-active bifunctional electrocatalysts for water splitting. *Energy and Environmental Science*, **2020**, 13, 545-553	35.4	99
596	Engineering Multifunctional Collaborative Catalytic Interface Enabling Efficient Hydrogen Evolution in All pH Range and Seawater. *Advanced Energy Materials*, **2019**, 9, 1901333	21.8	98
595	Hollow cages versus space-filling structures for medium-sized gold clusters: the spherical aromaticity of the Au50 cage. *Journal of Physical Chemistry A*, **2005**, 109, 9265-9	2.8	95
594	Melting behavior in ultrathin metallic nanowires. *Physical Review B*, **2002**, 66,	3.3	95
593	Amorphous structural models for graphene oxides. *Carbon*, **2012**, 50, 1690-1698	10.4	93
592	Screening and Design of Novel 2D Ferromagnetic Materials with High Curie Temperature above Room Temperature. *ACS Applied Materials & Interfaces*, **2018**, 10, 39032-39039	9.5	91
591	Oxidation Resistance of Monolayer Group-IV Monochalcogenides. *ACS Applied Materials & Interfaces*, **2017**, 9, 12013-12020	9.5	88
590	Structure and structural evolution of () clusters using a genetic algorithm and density functional theory method. *Solid State Communications*, **2007**, 144, 174-179	1.6	86
589	Genetic Algorithms for the Geometry Optimization of Atomic and Molecular Clusters. *Journal of Computational and Theoretical Nanoscience*, **2004**, 1, 117-131	0.3	86
588	YN2 monolayer: Novel p-state Dirac half metal for high-speed spintronics. *Nano Research*, **2017**, 10, 1972-1979	10	82
587	Growth behavior and magnetic properties of SinFe (n=2□14) clusters. *Physical Review B*, **2006**, 73,	3.3	82
586	Discovery of a silicon-based ferrimagnetic wheel structure in V(x)Si(12)(-) (x = 1-3) clusters: photoelectron spectroscopy and density functional theory investigation. *Nanoscale*, **2014**, 6, 14617-21	7.7	76
585	Endohedrally Doped Cage Clusters. *Chemical Reviews*, **2020**, 120, 9021-9163	68.1	76
584	N-doped graphitic carbon materials hybridized with transition metals (compounds) for hydrogen evolution reaction: Understanding the synergistic effect from atomistic level. *Carbon*, **2018**, 133, 260-266	10.4	75
583	A new phase diagram of water under negative pressure: The rise of the lowest-density clathrate s-III. *Science Advances*, **2016**, 2, e1501010	14.3	75
582	Lateral heterostructures of monolayer group-IV monochalcogenides: band alignment and electronic properties. *Journal of Materials Chemistry C*, **2017**, 5, 3788-3795	7.1	73
581	Complete Spin Polarization for a Carbon Nanotube with an Adsorbed Atomic Transition-Metal Chain. *Nano Letters*, **2004**, 4, 561-563	11.5	73
580	Structural and vibrational properties of solid nitromethane under high pressure by density functional theory. *Journal of Chemical Physics*, **2006**, 124, 124501	3.9	72

579	Shuttle inhibition by chemical adsorption of lithium polysulfides in B and N co-doped graphene for Li-S batteries. *Physical Chemistry Chemical Physics*, **2016**, 18, 25241-25248	3.6	72
578	Magnetic properties of atomic clusters and endohedral metallofullerenes. *Coordination Chemistry Reviews*, **2015**, 289-290, 315-340	23.2	69
577	Tailorable acceptor C(60-n)B(n) and donor C(60-m)N(m) pairs for molecular electronics. *Physical Review Letters*, **2003**, 90, 206602	7.4	69
576	2D Boron Sheets: Structure, Growth, and Electronic and Thermal Transport Properties. *Advanced Functional Materials*, **2020**, 30, 1904349	15.6	69
575	Intercalation and diffusion of lithium ions in a carbon nanotube bundle by ab initio molecular dynamics simulations. *Energy and Environmental Science*, **2011**, 4, 1379	35.4	68
574	Energetics and electronic structures of AlN nanotubes/wires and their potential application as ammonia sensors. *Nanotechnology*, **2007**, 18, 424023	3.4	67
573	Atomic structures and covalent-to-metallic transition of lead clusters Pbn(n=2□2). *Physical Review A*, **2005**, 71,	2.6	67
572	Quantum transport properties of ultrathin silver nanowires. *Nanotechnology*, **2003**, 14, 501-504	3.4	67
571	Electronic and photonic properties of doped carbon nanotubes. *Journal of Nanoscience and Nanotechnology*, **2003**, 3, 459-78	1.3	67
570	Engineering the electronic structure of single-walled carbon nanotubes by chemical functionalization. *ChemPhysChem*, **2005**, 6, 598-601	3.2	67
569	Band alignment of two-dimensional lateral heterostructures. *2D Materials*, **2017**, 4, 015038	5.9	66
568	Multilevel Hollow MXene Tailored Low-Pt Catalyst for Efficient Hydrogen Evolution in Full-pH Range and Seawater. *Advanced Functional Materials*, **2020**, 30, 1910028	15.6	66
567	Ni□a binary bulk metallic glasses. *Scripta Materialia*, **2010**, 63, 178-180	5.6	66
566	Body-centered tetragonal B2N2: a novel sp3 bonding boron nitride polymorph. *Physical Chemistry Chemical Physics*, **2011**, 13, 14565-70	3.6	65
565	Exceptional Electrochemical HER Performance with Enhanced Electron Transfer between Ru Nanoparticles and Single Atoms Dispersed on a Carbon Substrate. *Angewandte Chemie - International Edition*, **2021**, 60, 16044-16050	16.4	65
564	A new class of epitaxial porphyrin metal□rganic framework thin films with extremely high photocarrier generation efficiency: promising materials for all-solid-state solar cells. *Journal of Materials Chemistry A*, **2016**, 4, 12739-12747	13	64
563	Alloying effect on the elastic properties of refractory high-entropy alloys. *Materials and Design*, **2017**, 114, 243-252	8.1	64
562	Atomic and electronic structures of fluorinated BN nanotubes: computational study. *Journal of Physical Chemistry B*, **2006**, 110, 25678-85	3.4	64

561	Melting behavior of ultrathin titanium nanowires. *Physical Review B*, **2003**, 67,	3.3	64
560	First-principles calculations of structural, electronic, vibrational, and magnetic properties of C60 and C48N12: A comparative study. *Journal of Chemical Physics*, **2003**, 118, 8621-8635	3.9	64
559	Structures and electronic properties of symmetric and nonsymmetric graphene grain boundaries. *Carbon*, **2013**, 55, 151-159	10.4	63
558	High-pressure behavior of crystalline FOX-7 by density functional theory calculations. *Computational Materials Science*, **2008**, 42, 698-703	3.2	63
557	An exchange intercalation mechanism for the formation of a two-dimensional Si structure underneath graphene. *Nano Research*, **2012**, 5, 352-360	10	62
556	Boron fullerenes with 32–36 atoms: Irregular cage configurations and electronic properties. *Chemical Physics Letters*, **2010**, 501, 16-19	2.5	62
555	Inverse Capacity Growth and Pocket Effect in SnS Semifilled Carbon Nanotube Anode. *ACS Nano*, **2018**, 12, 8037-8047	16.7	61
554	Band Gap Modulated by Electronic Superlattice in Blue Phosphorene. *ACS Nano*, **2018**, 12, 5059-5065	16.7	61
553	Boron Nitride Nanotubes for Ammonia Synthesis: Activation by Filling Transition Metals. *Journal of the American Chemical Society*, **2020**, 142, 308-317	16.4	61
552	B28: the smallest all-boron cage from an ab initio global search. *Nanoscale*, **2015**, 7, 15086-90	7.7	60
551	The stability and electronic structure of single-walled ZnO nanotubes by density functional theory. *Nanotechnology*, **2007**, 18, 345706	3.4	60
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549	Stabilization of fullerene-like boron cages by transition metal encapsulation. *Nanoscale*, **2015**, 7, 10482-9	7.7	59
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547	Comprehensive genetic algorithm for ab initio global optimisation of clusters. *Molecular Simulation*, **2016**, 42, 809-819	2	59
546	Chemical environment and magnetic moment effects on point defect formations in CoCrNi-based concentrated solid-solution alloys. *Acta Materialia*, **2020**, 187, 122-134	8.4	57
545	A novel CuTi-containing catalyst derived from hydrotalcite-like compounds for selective catalytic reduction of NO with C3H6 under lean-burn conditions. *Journal of Catalysis*, **2014**, 309, 268-279	7.3	57
544	Distinct properties of single-wall carbon nanotubes with monovalent sidewall additions. *Nanotechnology*, **2005**, 16, 635-638	3.4	57

543	Cage and tube structures of medium-sized zinc oxide clusters (ZnO)n (n=24, 28, 36, and 48). *Journal of Chemical Physics*, **2008**, 128, 144710	3.9	56
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538	MXene nanoribbons as electrocatalysts for the hydrogen evolution reaction with fast kinetics. *Physical Chemistry Chemical Physics*, **2018**, 20, 19390-19397	3.6	53
537	Eighteen functional monolayer metal oxides: wide bandgap semiconductors with superior oxidation resistance and ultrahigh carrier mobility. *Nanoscale Horizons*, **2019**, 4, 592-600	10.8	51
536	Structure and magnetic properties of Co-Cu bimetallic clusters. *Physical Review B*, **2002**, 66,	3.3	51
535	Structural and Electronic Properties of Interfaces in Graphene and Hexagonal Boron Nitride Lateral Heterostructures. *Chemistry of Materials*, **2016**, 28, 5022-5028	9.6	51
534	Structures and Electronic Properties of V3Sin (n = 3–14) Clusters: A Combined Ab Initio and Experimental Study. *Journal of Physical Chemistry C*, **2015**, 119, 10987-10994	3.8	50
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530	Effect of surface Lewis acidity on selective catalytic reduction of NO by C3H6 over calcined hydrotalcite. *Applied Catalysis A: General*, **2013**, 451, 176-183	5.1	49
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528	Structures and electronic properties of ultrathin titanium nanowires. *Journal of Physics Condensed Matter*, **2001**, 13, L403-L408	1.8	49
527	Cooperative Electron-Phonon Coupling and Buckled Structure in Germanene on Au(111). *ACS Nano*, **2017**, 11, 3553-3559	16.7	48
526	Operando Revealing Dynamic Reconstruction of NiCo Carbonate Hydroxide for High-Rate Energy Storage. *Joule*, **2020**, 4, 673-687	27.8	48

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524	Phosphorus quantum dots as visible-light photocatalyst for water splitting. *Computational Materials Science*, **2017**, 130, 56-63	3.2	47
523	Reverse-Graded 2D Ruddlesden□Popper Perovskites for Efficient Air-Stable Solar Cells. *Advanced Energy Materials*, **2019**, 9, 1900612	21.8	47
522	First-principles study of molecular hydrogen dissociation on doped Al12X (X = B, Al, C, Si, P, Mg, and Ca) clusters. *Journal of Computational Chemistry*, **2009**, 30, 2509-14	3.5	46
521	MBenes: emerging 2D materials as efficient electrocatalysts for the nitrogen reduction reaction. *Nanoscale Horizons*, **2020**, 5, 1106-1115	10.8	45
520	Hybrids of PtRu Nanoclusters and Black Phosphorus Nanosheets for Highly Efficient Alkaline Hydrogen Evolution Reaction. *ACS Catalysis*, **2019**, 9, 10870-10875	13.1	45
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515	Structures and Magnetic Properties of MoS2 Grain Boundaries with Antisite Defects. *Journal of Physical Chemistry C*, **2017**, 121, 12261-12269	3.8	43
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512	GeAs and SiAs monolayers: Novel 2D semiconductors with suitable band structures. *Physica E: Low-Dimensional Systems and Nanostructures*, **2018**, 95, 149-153	3	43
511	Pressure-induced metallization in solid boron. *Physical Review B*, **2002**, 66,	3.3	43
510	Atomic structures and electronic properties of small Au□Ag binary clusters: Effects of size and composition. *Computational and Theoretical Chemistry*, **2012**, 993, 36-44	2	42
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506	Structural, electronic, and magnetic properties of heterofullerene C48B12. *Chemical Physics Letters*, **2003**, 375, 445-451	2.5	42
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490	Electronic Structures of Germanene on MoS2: Effect of Substrate and Molecular Adsorption. *Journal of Physical Chemistry C*, **2016**, 120, 21691-21698	3.8	36

489	He-induced vacancy formation in bcc Fe solid from first-principles simulation. *Journal of Nuclear Materials*, **2014**, 444, 147-152	3.3	36
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