Xi Zhu

List of Publications by Year in Descending Order

101 papers	3,482 citations	28 h-index	58 g-index
110 ext. papers	4,155 ext. citations	7.6 avg, IF	5.54 L-index

#	Paper	IF	Citations
101	Regulating Optical Activity and Anisotropic Second-Harmonic Generation in Zero-Dimensional Hybrid Copper Halides.. *Nano Letters*, **2022**,	11.5	5
100	Geometry Orbital of Deep Learning (GOODLE): A uniform carbon potential. *Carbon*, **2022**, 186, 313-319	10.4	1
99	Chiroptical Transitions of Enantiomeric Ligand-Activated Nickel Oxides.. *Small*, **2022**, e2107570	11	0
98	Tensor Network-Encrypted Physical Anti-counterfeiting Passport for Digital Twin Authentication. *ACS Applied Materials & Interfaces*, **2021**,	9.5	2
97	In Situ Determination of Polaron-Mediated Ultrafast Electron Trapping in Rutile TiO Nanorod Photoanodes. *Journal of Physical Chemistry Letters*, **2021**, 12, 10815-10822	6.4	6
96	Host/Guest Nanostructured Photoanodes Integrated with Targeted Enhancement Strategies for Photoelectrochemical Water Splitting. *Advanced Science*, **2021**, e2103744	13.6	6
95	Constructing spin pathways in LaCoO3 by Mn substitution to promote oxygen evolution reaction. *Applied Physics Letters*, **2021**, 119, 163902	3.4	2
94	Unraveling the Excitonic Transition and Associated Dynamics in Confined Long Linear Carbon Chains with Time-Resolved Resonance Raman Scattering. *Laser and Photonics Reviews*, **2021**, 15, 2100259	8.3	2
93	Gold Nanoparticle-Based Nanoengines for Light-Induced Plasmonic Bubble Generation. *ACS Applied Nano Materials*, **2021**, 4, 18-23	5.6	0
92	Giant Optical Activity and Second Harmonic Generation in 2D Hybrid Copper Halides. *Angewandte Chemie - International Edition*, **2021**, 60, 8441-8445	16.4	21
91	Giant Optical Activity and Second Harmonic Generation in 2D Hybrid Copper Halides. *Angewandte Chemie*, **2021**, 133, 8522-8526	3.6	5
90	Toward Programmable Moir□Computation. *Advanced Theory and Simulations*, **2021**, 4, 2100063	3.5	
89	Essentiality of the Basis Function in Deep Learning Physical Chemistry Properties. *Journal of Physical Chemistry Letters*, **2021**, 12, 6330-6335	6.4	
88	Theoretical predictions of two new chiral solid carbon oxides. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2021**, 385, 126941	2.3	1
87	Two predicted two-dimensional BCN structures: A first-principles study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 125, 114413	3	2
86	Toward Plant Energy Harvesting for 5G Signal Amplification. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 1099-1104	8.3	3
85	Catalyst deep neural networks (Cat-DNNs) in singlet fission property prediction. *Physical Chemistry Chemical Physics*, **2021**, 23, 20835-20840	3.6	1

84	Machine-learning-assisted low dielectric constant polymer discovery. *Materials Chemistry Frontiers*, **2021**, 5, 3823-3829	7.8	5
83	Metal-to-ligand charge transfer chirality-based sensing of mercury ions. *Photonics Research*, **2021**, 9, 213	6	0
82	Designing and Implementing VR2E2C, a Virtual Reality Remote Education for Experimental Chemistry System. *Journal of Chemical Education*, **2021**, 98, 2720-2725	2.4	3
81	The Origin of Magic Angle in Twisted Bilayer Graphene is Heisenberg's Uncertainty Principle. *Journal of Physical Chemistry Letters*, **2021**, 12, 9124-9131	6.4	0
80	QM-symex, update of the QM-sym database with excited state information for 173 kilo molecules. *Scientific Data*, **2020**, 7, 400	8.2	6
79	Effect of graphene quantum dot size on plant growth. *Nanoscale*, **2020**, 12, 15045-15049	7.7	13
78	Metal-to-Ligand Charge Transfer Chirality Sensing of d-Glucose Assisted with GOX-Based Enzymatic Reaction. *Advanced Materials Technologies*, **2020**, 5, 2000138	6.8	2
77	Hp-C17: A novel carbon allotrope with an all-sp3 network. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2020**, 384, 126379	2.3	3
76	Toward "On-Demand" Materials Synthesis and Scientific Discovery through Intelligent Robots. *Advanced Science*, **2020**, 7, 1901957	13.6	27
75	Theoretical investigations of a new two-dimensional semiconducting boron-carbon-nitrogen structure.. *RSC Advances*, **2020**, 10, 3424-3428	3.7	2
74	A prediction of a new porous metallic carbon allotrope with an sp2 hybridized network: cP-C24. *Solid State Sciences*, **2020**, 105, 106247	3.4	5
73	Eradication of tumor growth by delivering novel photothermal selenium-coated tellurium nanoheterojunctions. *Science Advances*, **2020**, 6, eaay6825	14.3	62
72	Autonomous discovery of optically active chiral inorganic perovskite nanocrystals through an intelligent cloud lab. *Nature Communications*, **2020**, 11, 2046	17.4	28
71	MXenes: focus on optical and electronic properties and corresponding applications. *Nanophotonics*, **2020**, 9, 1601-1620	6.3	31
70	CP-C20, a new metallic cubic carbon allotrope with an sp2 network. *Journal of Solid State Chemistry*, **2020**, 283, 121136	3.3	12
69	Interface modulation of BiVO4 based photoanode with Bi(III)Bi(V)O4 for enhanced solar water splitting. *Journal of Catalysis*, **2020**, 391, 513-521	7.3	5
68	The Blockchain Integrated Automatic Experiment Platform (BiaeP). *Journal of Physical Chemistry Letters*, **2020**, 11, 9995-10000	6.4	2
67	Symmetrical Graph Neural Network for Quantum Chemistry with Dual Real and Momenta Space. *Journal of Physical Chemistry A*, **2020**, 124, 6945-6953	2.8	11

66	Ligand-Induced Chirality in Asymmetric CdSe/CdS Nanostructures: A Close Look at Chiral Tadpoles. *ACS Nano*, **2020**, 14, 10346-10358	16.7	13
65	Chiral Transition Metal Oxides: Synthesis, Chiral Origins, and Perspectives. *Advanced Materials*, **2020**, 32, e1905585	24	15
64	Causal Inference Machine Learning Leads Original Experimental Discovery in CdSe/CdS Core/Shell Nanoparticles. *Journal of Physical Chemistry Letters*, **2020**, 11, 7232-7238	6.4	5
63	Phillips-Inspired Machine Learning for Band Gap and Exciton Binding Energy Prediction. *Journal of Physical Chemistry Letters*, **2019**, 10, 5640-5646	6.4	14
62	M-C21, an anti-ferromagnetic carbon bulk materials. *Solid State Communications*, **2019**, 302, 113707	1.6	1
61	Theoretical investigations of a new two-dimensional carbon allotrope: hP-C23-2D. *Computational Materials Science*, **2019**, 167, 8-12	3.2	11
60	Universal Scaling Law for Methane Capture Quantity in Metal□Organic Frameworks. *Advanced Theory and Simulations*, **2019**, 2, 1800170	3.5	2
59	Chiral CdSe nanoplatelets as an ultrasensitive probe for lead ion sensing. *Nanoscale*, **2019**, 11, 9327-9334	7.7	21
58	Manipulation of conjugation to stabilize N redox-active centers for the design of high-voltage organic battery cathode. *Energy Storage Materials*, **2019**, 16, 236-242	19.4	57
57	Engineering Lateral Heterojunction of Selenium-Coated Tellurium Nanomaterials toward Highly Efficient Solar Desalination. *Advanced Science*, **2019**, 6, 1900531	13.6	25
56	Universal Scaling of Excitons in Quasi One-Dimensional Carbon and Boron Nitride Allotropes. *Journal of Physical Chemistry C*, **2019**, 123, 25373-25378	3.8	
55	QM-sym, a symmetrized quantum chemistry database of 135 kilo molecules. *Scientific Data*, **2019**, 6, 213	8.2	9
54	The scaling of the ligand concentration and Soret effect induced phase transition in CsPbBr3 perovskite quantum dots. *Journal of Materials Chemistry A*, **2019**, 7, 27241-27246	13	5
53	Orbital-dependent redox potential regulation of quinone derivatives for electrical energy storage.. *RSC Advances*, **2019**, 9, 5164-5173	3.7	7
52	Lithium Clustering during the Lithiation/Delithiation Process in LiFePO Olivine-Structured Materials. *ACS Omega*, **2019**, 4, 20612-20617	3.9	2
51	A new two-dimensional semiconducting carbon allotrope: A first-principles study. *Carbon*, **2019**, 143, 517-522	10.4	31
50	Superbound Excitons in 2D Phosphorene Oxides. *Journal of Physical Chemistry A*, **2019**, 123, 21-25	2.8	2
49	Hexaoxaadamantane-Based Solid State Carbon Oxides. *ACS Applied Energy Materials*, **2019**, 2, 152-157	6.1	

48	CI24-Si: a Semiconducting Silicon Phase with an All-sp3 Bonding Network. *ChemistrySelect*, **2018**, 3, 451-455	1.8	7
47	TE-C36 carbon: a new semiconducting phase with an all-sp bonding network.. *RSC Advances*, **2018**, 8, 1846-1851	3.7	17
46	Tunable Chiroptical Properties from the Plasmonic Band to Metal□Ligand Charge Transfer Band of Cysteine-Capped Molybdenum Oxide Nanoparticles. *Angewandte Chemie*, **2018**, 130, 10393-10397	3.6	12
45	Black-phosphorus-analogue tin monosulfide: an emerging optoelectronic two-dimensional material for high-performance photodetection with improved stability under ambient/harsh conditions. *Journal of Materials Chemistry C*, **2018**, 6, 9582-9593	7.1	112
44	A New Metallic Porous Carbon Phase tP-C12 with an sp2-sp3 Bonding Network: A First-Principle Calculation. *ChemistrySelect*, **2018**, 3, 8402-8406	1.8	3
43	fvs-Si48: a direct bandgap silicon allotrope. *Physical Chemistry Chemical Physics*, **2018**, 20, 26091-26097	3.6	6
42	Ultrathin Metal□Organic Framework: An Emerging Broadband Nonlinear Optical Material for Ultrafast Photonics. *Advanced Optical Materials*, **2018**, 6, 1800561	8.1	214
41	Two-Dimensional Lead Monoxide: Facile Liquid Phase Exfoliation, Excellent Photoresponse Performance, and Theoretical Investigation. *ACS Photonics*, **2018**, 5, 5055-5067	6.3	31
40	AIR-Chem: Authentic Intelligent Robotics for Chemistry. *Journal of Physical Chemistry A*, **2018**, 122, 9142-9148	2.8	22
39	Optically Active CdSe-Dot/CdS-Rod Nanocrystals with Induced Chirality and Circularly Polarized Luminescence. *ACS Nano*, **2018**, 12, 5341-5350	16.7	73
38	Tunable Chiroptical Properties from the Plasmonic Band to Metal-Ligand Charge Transfer Band of Cysteine-Capped Molybdenum Oxide Nanoparticles. *Angewandte Chemie - International Edition*, **2018**, 57, 10236-10240	16.4	35
37	Chiral Pentagon Only Diamond-like Structures. *Journal of Physical Chemistry C*, **2017**, 121, 13810-13815	3.8	13
36	Pseudo-topotactic conversion of carbon nanotubes to T-carbon nanowires under picosecond laser irradiation in methanol. *Nature Communications*, **2017**, 8, 683	17.4	130
35	Porous CY carbon: a new semiconducting phase with an sp1□p2□p3 bonding network. *RSC Advances*, **2016**, 6, 112035-112039	3.7	7
34	Phosphorene: from theory to applications. *Nature Reviews Materials*, **2016**, 1,	73.3	571
33	Electronic and optical properties of surface hydrogenated armchair graphene nanoribbons: a theoretical study. *RSC Advances*, **2016**, 6, 11786-11794	3.7	7
32	CTAB-Influenced Electrochemical Dissolution of Silver Dendrites. *Langmuir*, **2016**, 32, 3601-7	4	16
31	Nanodroplet-Mediated Assembly of Platinum Nanoparticle Rings in Solution. *Nano Letters*, **2016**, 16, 1092-6	11.5	31

30	Scaling Law of Exciton Properties in the Surface Hydrogenated Armchair Graphene Nanoribbon. *ChemistrySelect*, **2016**, 1, 1658-1661	1.8	6
29	Magnetism in graphene oxide induced by epoxy groups. *Applied Physics Letters*, **2015**, 106, 172402	3.4	31
28	Design of an oscillator with low phase noise and medium output power in a 0.25 μm GaN-on-SiC high electron-mobility transistors technology. *IET Microwaves, Antennas and Propagation*, **2015**, 9, 795-801	1.6	7
27	Vibrational spectrum renormalization by enforced coupling across the van der Waals gap between MoS2 and WS2 monolayers. *Physical Review B*, **2015**, 92,	3.3	19
26	Excitonic Character in Optical Properties of Tetrahedral CdX (X = S, Se, Te) Clusters. *Journal of Physical Chemistry C*, **2015**, 119, 29171-29177	3.8	14
25	Exciton characteristics in graphene epoxide. *ACS Nano*, **2014**, 8, 1284-9	16.7	27
24	Textured fluorapatite bonded to calcium sulphate strengthen stomatopod raptorial appendages. *Nature Communications*, **2014**, 5, 3187	17.4	78
23	Merging of metal nanoparticles driven by selective wettability of silver nanostructures. *Nature Communications*, **2014**, 5, 2994	17.4	47
22	Computed and Experimental Absorption Spectra of the Perovskite CH3NH3PbI3. *Journal of Physical Chemistry Letters*, **2014**, 5, 3061-5	6.4	80
21	Excitonic Photoluminescence from Nanodisc States in Graphene Oxides. *Journal of Physical Chemistry Letters*, **2014**, 5, 1754-9	6.4	47
20	Bonding pathways of gold nanocrystals in solution. *Nano Letters*, **2014**, 14, 6639-43	11.5	65
19	Quantum confinement-induced tunable exciton states in graphene oxide. *Scientific Reports*, **2013**, 3, 2250	4.9	47
18	Ultrafast carrier phonon dynamics in NaOH-reacted graphite oxide film. *Applied Physics Letters*, **2012**, 101, 021604	3.4	12
17	Scaling of excitons in graphene nanoribbons with armchair shaped edges. *Journal of Physical Chemistry A*, **2011**, 115, 11998-2003	2.8	54
16	Excitons of Edge and Surface Functionalized Graphene Nanoribbons. *Journal of Physical Chemistry C* , **2010**, 114, 17257-17262	3.8	33
15	Magnetism in hybrid carbon nanostructures: Nanobuds. *Physical Review B*, **2009**, 79,	3.3	28
14	Surfactant-Assisted Etching in Biomimetic Mineralization of Ferric Phosphate. *Chemistry of Materials*, **2008**, 20, 3959-3964	9.6	17
13	Surfactant-free synthesis of hyperbranched monoclinic bismuth vanadate and its applications in photocatalysis, gas sensing, and lithium-ion batteries. *Chemistry - A European Journal*, **2008**, 14, 1601-6	4.8	179

List of Publications

12	Fabrication of Micrometer-Scaled Hierarchical Tubular Structures of CuS Assembled by Nanoflake-built Microspheres Using an In Situ Formed Cu(I) Complex as a Self-Sacrificed Template. *Crystal Growth and Design*, **2007**, 7, 1256-1261	3.5	83
11	Synthesis and Optical Properties of □BaB2O4 Network-Like Nanostructures. *European Journal of Inorganic Chemistry*, **2007**, 2007, 1829-1834	2.3	25
10	Synthesis of novel Y-junction hollow carbon nanotrees. *Carbon*, **2007**, 45, 1566-1570	10.4	27
9	Multiarmed tubular selenium with potentially unique electrical properties: solution-phase synthesis and first-principles calculation. *Small*, **2007**, 3, 101-5	11	13
8	Large-scale synthesis of titanate and anatase tubular hierarchitectures. *Small*, **2007**, 3, 1518-22	11	68
7	Synthesis, Growth Mechanism, and Work Function at Highly Oriented {001} Surfaces of Bismuth Sulfide Microbelts. *Journal of Physical Chemistry C*, **2007**, 111, 12145-12148	3.8	28
6	Bamboolike carbon nitride nanotubes (C9N5H3): Atomic-scale construction, synthesis and lithium battery applications. *Applied Physics Letters*, **2007**, 90, 113116	3.4	8
5	Necklace-like hollow carbon nanospheres from the pentagon-including reactants: synthesis and electrochemical properties. *Inorganic Chemistry*, **2006**, 45, 8543-50	5.1	61
4	Synthesis of hematite (alpha-Fe2O3) nanorods: diameter-size and shape effects on their applications in magnetism, lithium ion battery, and gas sensors. *Journal of Physical Chemistry B*, **2006**, 110, 17806-12	3.4	566
3	Machine Learning-Assisted Discovery of High-Voltage Organic Materials for Rechargeable Batteries. *Journal of Physical Chemistry C*,	3.8	4
2	Robots Built Robots: Nanorobots Customized by Intelligent Robot. *Crystal Growth and Design*,	3.5	1
1	Single Pd□x Sites In Situ Coordinated on CdS Surface as Efficient Hydrogen Autotransfer Shuttles for Highly Selective Visible-Light-Driven C□N Coupling. *ACS Catalysis*,4481-4490	13.1	3