

Xi Zhu

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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	Phosphorene: from theory to applications. <i>Nature Reviews Materials</i> , 2016 , 1,	73.3	571
100	Synthesis of hematite ($\alpha\text{-Fe}_2\text{O}_3$) nanorods: diameter-size and shape effects on their applications in magnetism, lithium ion battery, and gas sensors. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 17806-12	3.4	566
99	Ultrathin MetalOrganic Framework: An Emerging Broadband Nonlinear Optical Material for Ultrafast Photonics. <i>Advanced Optical Materials</i> , 2018 , 6, 1800561	8.1	214
98	Surfactant-free synthesis of hyperbranched monoclinic bismuth vanadate and its applications in photocatalysis, gas sensing, and lithium-ion batteries. <i>Chemistry - A European Journal</i> , 2008 , 14, 1601-6	4.8	179
97	Pseudo-topotactic conversion of carbon nanotubes to T-carbon nanowires under picosecond laser irradiation in methanol. <i>Nature Communications</i> , 2017 , 8, 683	17.4	130
96	Black-phosphorus-analogue tin monosulfide: an emerging optoelectronic two-dimensional material for high-performance photodetection with improved stability under ambient/harsh conditions. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 9582-9593	7.1	112
95	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. <i>Crystal Growth and Design</i> , 2007 , 7, 1256-1261	3.5	83
94	Computed and Experimental Absorption Spectra of the Perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 3061-5	6.4	80
93	Textured fluorapatite bonded to calcium sulphate strengthen stomatopod raptorial appendages. <i>Nature Communications</i> , 2014 , 5, 3187	17.4	78
92	Optically Active CdSe-Dot/CdS-Rod Nanocrystals with Induced Chirality and Circularly Polarized Luminescence. <i>ACS Nano</i> , 2018 , 12, 5341-5350	16.7	73
91	Large-scale synthesis of titanate and anatase tubular hierarchitectures. <i>Small</i> , 2007 , 3, 1518-22	11	68
90	Bonding pathways of gold nanocrystals in solution. <i>Nano Letters</i> , 2014 , 14, 6639-43	11.5	65
89	Eradication of tumor growth by delivering novel photothermal selenium-coated tellurium nanoheterojunctions. <i>Science Advances</i> , 2020 , 6, eaay6825	14.3	62
88	Necklace-like hollow carbon nanospheres from the pentagon-including reactants: synthesis and electrochemical properties. <i>Inorganic Chemistry</i> , 2006 , 45, 8543-50	5.1	61
87	Manipulation of conjugation to stabilize N redox-active centers for the design of high-voltage organic battery cathode. <i>Energy Storage Materials</i> , 2019 , 16, 236-242	19.4	57
86	Scaling of excitons in graphene nanoribbons with armchair shaped edges. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 11998-2003	2.8	54
85	Merging of metal nanoparticles driven by selective wettability of silver nanostructures. <i>Nature Communications</i> , 2014 , 5, 2994	17.4	47

84	Excitonic Photoluminescence from Nanodisc States in Graphene Oxides. <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 1754-9	6.4	47
83	Quantum confinement-induced tunable exciton states in graphene oxide. <i>Scientific Reports</i> , 2013 , 3, 2250	4.9	47
82	Tunable Chiroptical Properties from the Plasmonic Band to Metal-Ligand Charge Transfer Band of Cysteine-Capped Molybdenum Oxide Nanoparticles. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 10236-10240	16.4	35
81	Excitons of Edge and Surface Functionalized Graphene Nanoribbons. <i>Journal of Physical Chemistry C</i> , 2010 , 114, 17257-17262	3.8	33
80	Magnetism in graphene oxide induced by epoxy groups. <i>Applied Physics Letters</i> , 2015 , 106, 172402	3.4	31
79	Nanodroplet-Mediated Assembly of Platinum Nanoparticle Rings in Solution. <i>Nano Letters</i> , 2016 , 16, 1092-6	11.5	31
78	MXenes: focus on optical and electronic properties and corresponding applications. <i>Nanophotonics</i> , 2020 , 9, 1601-1620	6.3	31
77	A new two-dimensional semiconducting carbon allotrope: A first-principles study. <i>Carbon</i> , 2019 , 143, 517-522	10.4	31
76	Two-Dimensional Lead Monoxide: Facile Liquid Phase Exfoliation, Excellent Photoresponse Performance, and Theoretical Investigation. <i>ACS Photonics</i> , 2018 , 5, 5055-5067	6.3	31
75	Autonomous discovery of optically active chiral inorganic perovskite nanocrystals through an intelligent cloud lab. <i>Nature Communications</i> , 2020 , 11, 2046	17.4	28
74	Magnetism in hybrid carbon nanostructures: Nanobuds. <i>Physical Review B</i> , 2009 , 79,	3.3	28
73	Synthesis, Growth Mechanism, and Work Function at Highly Oriented {001} Surfaces of Bismuth Sulfide Microbelts. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 12145-12148	3.8	28
72	Toward "On-Demand" Materials Synthesis and Scientific Discovery through Intelligent Robots. <i>Advanced Science</i> , 2020 , 7, 1901957	13.6	27
71	Exciton characteristics in graphene epoxide. <i>ACS Nano</i> , 2014 , 8, 1284-9	16.7	27
70	Synthesis of novel Y-junction hollow carbon nanotrees. <i>Carbon</i> , 2007 , 45, 1566-1570	10.4	27
69	Engineering Lateral Heterojunction of Selenium-Coated Tellurium Nanomaterials toward Highly Efficient Solar Desalination. <i>Advanced Science</i> , 2019 , 6, 1900531	13.6	25
68	Synthesis and Optical Properties of EBaB_2O_4 Network-Like Nanostructures. <i>European Journal of Inorganic Chemistry</i> , 2007 , 2007, 1829-1834	2.3	25
67	AIR-Chem: Authentic Intelligent Robotics for Chemistry. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 9142-9148	2.8	22

66	Chiral CdSe nanoplatelets as an ultrasensitive probe for lead ion sensing. <i>Nanoscale</i> , 2019 , 11, 9327-9334.	4.7	21
65	Giant Optical Activity and Second Harmonic Generation in 2D Hybrid Copper Halides. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 8441-8445	16.4	21
64	Vibrational spectrum renormalization by enforced coupling across the van der Waals gap between MoS ₂ and WS ₂ monolayers. <i>Physical Review B</i> , 2015 , 92,	3.3	19
63	TE-C36 carbon: a new semiconducting phase with an all-sp bonding network.. <i>RSC Advances</i> , 2018 , 8, 1846-1851	3.7	17
62	Surfactant-Assisted Etching in Biomimetic Mineralization of Ferric Phosphate. <i>Chemistry of Materials</i> , 2008 , 20, 3959-3964	9.6	17
61	CTAB-Influenced Electrochemical Dissolution of Silver Dendrites. <i>Langmuir</i> , 2016 , 32, 3601-7	4	16
60	Chiral Transition Metal Oxides: Synthesis, Chiral Origins, and Perspectives. <i>Advanced Materials</i> , 2020 , 32, e1905585	24	15
59	Phillips-Inspired Machine Learning for Band Gap and Exciton Binding Energy Prediction. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 5640-5646	6.4	14
58	Excitonic Character in Optical Properties of Tetrahedral CdX (X = S, Se, Te) Clusters. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 29171-29177	3.8	14
57	Chiral Pentagon Only Diamond-like Structures. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 13810-13815	3.8	13
56	Effect of graphene quantum dot size on plant growth. <i>Nanoscale</i> , 2020 , 12, 15045-15049	7.7	13
55	Multiarmed tubular selenium with potentially unique electrical properties: solution-phase synthesis and first-principles calculation. <i>Small</i> , 2007 , 3, 101-5	11	13
54	Ligand-Induced Chirality in Asymmetric CdSe/CdS Nanostructures: A Close Look at Chiral Tadpoles. <i>ACS Nano</i> , 2020 , 14, 10346-10358	16.7	13
53	Tunable Chiroptical Properties from the Plasmonic Band to Metal-Ligand Charge Transfer Band of Cysteine-Capped Molybdenum Oxide Nanoparticles. <i>Angewandte Chemie</i> , 2018 , 130, 10393-10397	3.6	12
52	Ultrafast carrier phonon dynamics in NaOH-reacted graphite oxide film. <i>Applied Physics Letters</i> , 2012 , 101, 021604	3.4	12
51	CP-C20, a new metallic cubic carbon allotrope with an sp ² network. <i>Journal of Solid State Chemistry</i> , 2020 , 283, 121136	3.3	12
50	Theoretical investigations of a new two-dimensional carbon allotrope: hP-C23-2D. <i>Computational Materials Science</i> , 2019 , 167, 8-12	3.2	11
49	Symmetrical Graph Neural Network for Quantum Chemistry with Dual Real and Momenta Space. <i>Journal of Physical Chemistry A</i> , 2020 , 124, 6945-6953	2.8	11

48	QM-sym, a symmetrized quantum chemistry database of 135 kilo molecules. <i>Scientific Data</i> , 2019 , 6, 2138.2	9
47	Bamboolike carbon nitride nanotubes (C ₉ N ₅ H ₃): Atomic-scale construction, synthesis and lithium battery applications. <i>Applied Physics Letters</i> , 2007 , 90, 113116	3.4 8
46	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. <i>IET Microwaves, Antennas and Propagation</i> , 2015 , 9, 795-801	1.6 7
45	Cl ₂₄ -Si: a Semiconducting Silicon Phase with an All-sp ³ Bonding Network. <i>ChemistrySelect</i> , 2018 , 3, 451-455	1.5 7
44	Porous CY carbon: a new semiconducting phase with an sp ^{1.8} p ^{2.2} sp ³ bonding network. <i>RSC Advances</i> , 2016 , 6, 112035-112039	3.7 7
43	Electronic and optical properties of surface hydrogenated armchair graphene nanoribbons: a theoretical study. <i>RSC Advances</i> , 2016 , 6, 11786-11794	3.7 7
42	Orbital-dependent redox potential regulation of quinone derivatives for electrical energy storage.. <i>RSC Advances</i> , 2019 , 9, 5164-5173	3.7 7
41	QM-symex, update of the QM-sym database with excited state information for 173 kilo molecules. <i>Scientific Data</i> , 2020 , 7, 400	8.2 6
40	fvs-Si ₄₈ : a direct bandgap silicon allotrope. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 26091-26097	3.6 6
39	In Situ Determination of Polaron-Mediated Ultrafast Electron Trapping in Rutile TiO Nanorod Photoanodes. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 10815-10822	6.4 6
38	Host/Guest Nanostructured Photoanodes Integrated with Targeted Enhancement Strategies for Photoelectrochemical Water Splitting. <i>Advanced Science</i> , 2021 , e2103744	13.6 6
37	Scaling Law of Exciton Properties in the Surface Hydrogenated Armchair Graphene Nanoribbon. <i>ChemistrySelect</i> , 2016 , 1, 1658-1661	1.8 6
36	A prediction of a new porous metallic carbon allotrope with an sp ² hybridized network: cP-C ₂₄ . <i>Solid State Sciences</i> , 2020 , 105, 106247	3.4 5
35	The scaling of the ligand concentration and Soret effect induced phase transition in CsPbBr ₃ perovskite quantum dots. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 27241-27246	13 5
34	Regulating Optical Activity and Anisotropic Second-Harmonic Generation in Zero-Dimensional Hybrid Copper Halides.. <i>Nano Letters</i> , 2022 ,	11.5 5
33	Interface modulation of BiVO ₄ based photoanode with Bi(III)Bi(V)O ₄ for enhanced solar water splitting. <i>Journal of Catalysis</i> , 2020 , 391, 513-521	7.3 5
32	Causal Inference Machine Learning Leads Original Experimental Discovery in CdSe/CdS Core/Shell Nanoparticles. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 7232-7238	6.4 5
31	Giant Optical Activity and Second Harmonic Generation in 2D Hybrid Copper Halides. <i>Angewandte Chemie</i> , 2021 , 133, 8522-8526	3.6 5

30	Machine-learning-assisted low dielectric constant polymer discovery. <i>Materials Chemistry Frontiers</i> , 2021 , 5, 3823-3829	7.8	5
29	Machine Learning-Assisted Discovery of High-Voltage Organic Materials for Rechargeable Batteries. <i>Journal of Physical Chemistry C</i> ,	3.8	4
28	Hp-C17: A novel carbon allotrope with an all-sp ³ network. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020 , 384, 126379	2.3	3
27	A New Metallic Porous Carbon Phase tP-C12 with an sp ² -sp ³ Bonding Network: A First-Principle Calculation. <i>ChemistrySelect</i> , 2018 , 3, 8402-8406	1.8	3
26	Toward Plant Energy Harvesting for 5G Signal Amplification. <i>ACS Sustainable Chemistry and Engineering</i> , 2021 , 9, 1099-1104	8.3	3
25	Designing and Implementing VR2E2C, a Virtual Reality Remote Education for Experimental Chemistry System. <i>Journal of Chemical Education</i> , 2021 , 98, 2720-2725	2.4	3
24	Single Pd ₃ Sites In Situ Coordinated on CdS Surface as Efficient Hydrogen Autotransfer Shuttles for Highly Selective Visible-Light-Driven C-N Coupling. <i>ACS Catalysis</i> , 4481-4490	13.1	3
23	Universal Scaling Law for Methane Capture Quantity in Metal-Organic Frameworks. <i>Advanced Theory and Simulations</i> , 2019 , 2, 1800170	3.5	2
22	Metal-to-Ligand Charge Transfer Chirality Sensing of d-Glucose Assisted with GOX-Based Enzymatic Reaction. <i>Advanced Materials Technologies</i> , 2020 , 5, 2000138	6.8	2
21	Theoretical investigations of a new two-dimensional semiconducting boron-carbon-nitrogen structure.. <i>RSC Advances</i> , 2020 , 10, 3424-3428	3.7	2
20	Tensor Network-Encrypted Physical Anti-counterfeiting Passport for Digital Twin Authentication. <i>ACS Applied Materials & Interfaces</i> , 2021 ,	9.5	2
19	Constructing spin pathways in LaCoO ₃ by Mn substitution to promote oxygen evolution reaction. <i>Applied Physics Letters</i> , 2021 , 119, 163902	3.4	2
18	Unraveling the Excitonic Transition and Associated Dynamics in Confined Long Linear Carbon Chains with Time-Resolved Resonance Raman Scattering. <i>Laser and Photonics Reviews</i> , 2021 , 15, 2100259	8.3	2
17	The Blockchain Integrated Automatic Experiment Platform (BiaeP). <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 9995-10000	6.4	2
16	Lithium Clustering during the Lithiation/Delithiation Process in LiFePO ₄ Olivine-Structured Materials. <i>ACS Omega</i> , 2019 , 4, 20612-20617	3.9	2
15	Superbound Excitons in 2D Phosphorene Oxides. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 21-25	2.8	2
14	Two predicted two-dimensional BCN structures: A first-principles study. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2021 , 125, 114413	3	2
13	M-C21, an anti-ferromagnetic carbon bulk materials. <i>Solid State Communications</i> , 2019 , 302, 113707	1.6	1

12	Geometry Orbital of Deep Learning (GOODLE): A uniform carbon potential. <i>Carbon</i> , 2022 , 186, 313-319	10.4	1
11	Theoretical predictions of two new chiral solid carbon oxides. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021 , 385, 126941	2.3	1
10	Catalyst deep neural networks (Cat-DNNs) in singlet fission property prediction. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 20835-20840	3.6	1
9	Robots Built Robots: Nanorobots Customized by Intelligent Robot. <i>Crystal Growth and Design</i> ,	3.5	1
8	Gold Nanoparticle-Based Nanoengines for Light-Induced Plasmonic Bubble Generation. <i>ACS Applied Nano Materials</i> , 2021 , 4, 18-23	5.6	0
7	Metal-to-ligand charge transfer chirality-based sensing of mercury ions. <i>Photonics Research</i> , 2021 , 9, 213	6	0
6	The Origin of Magic Angle in Twisted Bilayer Graphene is Heisenberg's Uncertainty Principle. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 9124-9131	6.4	0
5	Chiroptical Transitions of Enantiomeric Ligand-Activated Nickel Oxides.. <i>Small</i> , 2022 , e2107570	11	0
4	Universal Scaling of Excitons in Quasi One-Dimensional Carbon and Boron Nitride Allotropes. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 25373-25378	3.8	
3	Toward Programmable Moiré Computation. <i>Advanced Theory and Simulations</i> , 2021 , 4, 2100063	3.5	
2	Essentiality of the Basis Function in Deep Learning Physical Chemistry Properties. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 6330-6335	6.4	
1	Hexaoxadamantane-Based Solid State Carbon Oxides. <i>ACS Applied Energy Materials</i> , 2019 , 2, 152-157	6.1	