Zhenyu Li

List of Publications by Year
in descending order

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		22099	30848
201	11,904	59	102
papers	citations	h-index	g-index

202	202	202	13399
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Half-Metallicity in Edge-Modified Zigzag Graphene Nanoribbons. Journal of the American Chemical Society, 2008, 130, 4224-4225.	6.6	640
2	Epitaxial Growth of Single Layer Blue Phosphorus: A New Phase of Two-Dimensional Phosphorus. Nano Letters, 2016, 16, 4903-4908.	4.5	609
3	Low-Temperature Growth of Graphene by Chemical Vapor Deposition Using Solid and Liquid Carbon Sources. ACS Nano, 2011, 5, 3385-3390.	7.3	353
4	Single mode optofluidic distributed feedback dye laser. Optics Express, 2006, 14, 696.	1.7	335
5	How Graphene Is Cut upon Oxidation?. Journal of the American Chemical Society, 2009, 131, 6320-6321.	6.6	323
6	First-Principles Thermodynamics of Graphene Growth on Cu Surfaces. Journal of Physical Chemistry C, 2011, 115, 17782-17787.	1.5	317
7	Will zigzag graphene nanoribbon turn to half metal under electric field?. Applied Physics Letters, 2007, 91, .	1.5	299
8	Obtaining Two-Dimensional Electron Gas in Free Space without Resorting to Electron Doping: An Electride Based Design. Journal of the American Chemical Society, 2014, 136, 13313-13318.	6.6	280
9	Bipolar magnetic semiconductors: a new class of spintronics materials. Nanoscale, 2012, 4, 5680.	2.8	241
10	Proposed Photosynthesis Method for Producing Hydrogen from Dissociated Water Molecules Using Incident Near-Infrared Light. Physical Review Letters, 2014, 112, 018301.	2.9	237
11	A first-principles study of gas adsorption on germanene. Physical Chemistry Chemical Physics, 2014, 16, 22495-22498.	1.3	232
12	Electronic structures of SiC nanoribbons. Journal of Chemical Physics, 2008, 129, 174114.	1.2	222
13	Silicene as a highly sensitive molecule sensor for NH3, NO and NO2. Physical Chemistry Chemical Physics, 2014, 16, 6957.	1.3	221
14	Oxygen molecule dissociation on carbon nanostructures with different types of nitrogen doping. Nanoscale, 2012, 4, 1184-1189.	2.8	220
15	A multi-color fast-switching microfluidic droplet dye laser. Lab on A Chip, 2009, 9, 2767.	3.1	177
16	Adsorption energies of molecular oxygen on Au clusters. Journal of Chemical Physics, 2004, 120, 9594-9600.	1.2	159
17	Mo2C nanoparticles embedded within bacterial cellulose-derived 3D N-doped carbon nanofiber networks for efficient hydrogen evolution. NPG Asia Materials, 2016, 8, e288-e288.	3.8	153
18	Site-specific photocatalytic splitting of methanol on TiO2(110). Chemical Science, 2010, 1, 575.	3.7	150

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19	Optofluidic dye lasers. Microfluidics and Nanofluidics, 2008, 4, 145-158.	1.0	143
20	Remarkable chemical adsorption of manganese-doped titanate for direct carbon dioxide electrolysis. Journal of Materials Chemistry A, 2014, 2, 6904-6915.	5.2	137
21	Half-metallicity in hybrid BCN nanoribbons. Journal of Chemical Physics, 2008, 129, 084712.	1.2	133
22	Electronic Structure Engineering via On-Plane Chemical Functionalization: A Comparison Study on Two-Dimensional Polysilane and Graphane. Journal of Physical Chemistry C, 2009, 113, 16741-16746.	1.5	133
23	Mechanically tunable optofluidic distributed feedback dye laser. Optics Express, 2006, 14, 10494.	1.7	128
24	Porous silicene as a hydrogen purification membrane. Physical Chemistry Chemical Physics, 2013, 15, 5753.	1.3	127
25	Pt Single Atoms Embedded in the Surface of Ni Nanocrystals as Highly Active Catalysts for Selective Hydrogenation of Nitro Compounds. Nano Letters, 2018, 18, 3785-3791.	4.5	127
26	Electron-phonon coupling in a boron-doped diamond superconductor. Physical Review B, 2004, 70, .	1.1	126
27	Paleomagnetic constraints on the Mesozoic drift of the Lhasa terrane (Tibet) from Gondwana to Eurasia. Geology, 2016, 44, 727-730.	2.0	118
28	Growth of Quasi-Free-Standing Single-Layer Blue Phosphorus on Tellurium Monolayer Functionalized Au(111). ACS Nano, 2017, 11, 4943-4949.	7.3	109
29	Single-Molecule Chemistry of Metal Phthalocyanine on Noble Metal Surfaces. Accounts of Chemical Research, 2010, 43, 954-962.	7.6	105
30	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2012, 116, 3142-3146.	1.5	103
31	Late Triassic paleolatitude of the Qiangtang block: Implications for the closure of the Paleo-Tethys Ocean. Earth and Planetary Science Letters, 2015, 424, 69-83.	1.8	98
32	Electronic and optical properties of graphene and graphitic ZnO nanocomposite structures. Journal of Chemical Physics, 2013, 138, 124706.	1.2	97
33	Helium separation via porous silicene based ultimate membrane. Nanoscale, 2013, 5, 9062.	2.8	96
34	Aerobic Oxidation of Cyclohexane on Catalysts Based on Twinned and Single-Crystal Au₇₅Pd₂₅ Bimetallic Nanocrystals. Nano Letters, 2015, 15, 2875-2880.	4.5	92
35	Structure of Graphene Oxide: Thermodynamics versus Kinetics. Journal of Physical Chemistry C, 2011, 115, 11991-11995.	1.5	91
36	The early Eocene rise of the Gonjo Basin, SE Tibet: From low desert to high forest. Earth and Planetary Science Letters, 2020, 543, 116312.	1.8	91

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37	Precursor Triggering Synthesis of Self-Coupled Sulfide Polymorphs with Enhanced Photoelectrochemical Properties. Journal of the American Chemical Society, 2016, 138, 12913-12919.	6.6	90
38	Oxidation states of graphene: Insights from computational spectroscopy. Journal of Chemical Physics, 2009, 131, 244505.	1.2	88
39	Lattice Mismatch Induced Nonlinear Growth of Graphene. Journal of the American Chemical Society, 2012, 134, 6045-6051.	6.6	88
40	Structural, electronic, and optical properties of hybrid silicene and graphene nanocomposite. Journal of Chemical Physics, 2013, 139, 154704.	1.2	84
41	Flexible packaging of solid-state integrated circuit chips with elastomeric microfluidics. Scientific Reports, 2013, 3, .	1.6	83
42	Single Faceted Two-Dimensional Mo₂C Electrocatalyst for Highly Efficient Nitrogen Fixation. ACS Catalysis, 2020, 10, 7864-7870.	5.5	80
43	The rise and demise of the Paleogene Central Tibetan Valley. Science Advances, 2022, 8, eabj0944.	4.7	80
44	Theoretical study of nitric oxide adsorption on Au clusters. Journal of Chemical Physics, 2004, 121, 2558.	1.2	78
45	Dithiocarbamate Anchoring in Molecular Wire Junctions:Â A First Principles Study. Journal of Physical Chemistry B, 2006, 110, 9893-9898.	1.2	78
46	Ratio-Controlled Synthesis of CuNi Octahedra and Nanocubes with Enhanced Catalytic Activity. Journal of the American Chemical Society, 2015, 137, 14027-14030.	6.6	75
47	Contrasting Structural Reconstructions, Electronic Properties, and Magnetic Orderings along Different Edges of Zigzag Transition Metal Dichalcogenide Nanoribbons. Nano Letters, 2017, 17, 1097-1101.	4.5	75
48	Nature of well-defined conductance of amine-anchored molecular junctions: Density functional calculations. Physical Review B, 2007, 76, .	1.1	74
49	Mechanisms of Graphene Growth on Metal Surfaces: Theoretical Perspectives. Small, 2014, 10, 2136-2150.	5.2	73
50	Carbon Dimers as the Dominant Feeding Species in Epitaxial Growth and Morphological Phase Transition of Graphene on Different Cu Substrates. Physical Review Letters, 2015, 114, 216102.	2.9	73
51	Communication: Coalescence of carbon atoms on Cu (111) surface: Emergence of a stable bridging-metal structure motif. Journal of Chemical Physics, 2010, 133, 071101.	1.2	72
52	MAGNETISM IN GRAPHENE SYSTEMS. Nano, 2008, 03, 433-442.	0.5	70
53	Graphene Thickness Control via Gas-Phase Dynamics in Chemical Vapor Deposition. Journal of Physical Chemistry C, 2012, 116, 10557-10562.	1.5	70
54	Is Mayenite without Clathrated Oxygen an Inorganic Electride?. Angewandte Chemie - International Edition, 2004, 43, 6479-6482.	7.2	68

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55	A first-principles prediction of two-dimensional superconductivity in pristine B2C single layers. Nanoscale, 2012, 4, 3032.	2.8	67
56	An early bird from Gondwana: Paleomagnetism of Lower Permian lavas from northern Qiangtang (Tibet) and the geography of the Paleo-Tethys. Earth and Planetary Science Letters, 2017, 475, 119-133.	1.8	67
57	Optofluidic evanescent dye laser based on a distributed feedback circular grating. Applied Physics Letters, 2009, 94, 161110.	1.5	66
58	Effects of nano- and microplastics on kidney: Physicochemical properties, bioaccumulation, oxidative stress and immunoreaction. Chemosphere, 2022, 288, 132631.	4.2	66
59	Descriptor-Based Design Principle for Two-Dimensional Single-Atom Catalysts: Carbon Dioxide Electroreduction. Journal of Physical Chemistry Letters, 2020, 11, 3481-3487.	2.1	65
60	Dominant Kinetic Pathways of Graphene Growth in Chemical Vapor Deposition: The Role of Hydrogen. Journal of Physical Chemistry C, 2017, 121, 25949-25955.	1.5	61
61	Low-order distributed feedback optofluidic dye laser with reduced threshold. Applied Physics Letters, 2009, 94, .	1.5	56
62	Hydrogenated bilayer wurtzite SiC nanofilms: a two-dimensional bipolar magnetic semiconductor material. Physical Chemistry Chemical Physics, 2013, 15, 497-503.	1.3	55
63	Antibody Quantum Dot Conjugates Developed via Copper-Free Click Chemistry for Rapid Analysis of Biological Samples Using a Microfluidic Microsphere Array System. Bioconjugate Chemistry, 2014, 25, 1272-1281.	1.8	55
64	A smartphone controlled handheld microfluidic liquid handling system. Lab on A Chip, 2014, 14, 4085-4092.	3.1	54
65	Diamondization of chemically functionalized graphene and grapheneâ€“BN bilayers. Physical Chemistry Chemical Physics, 2012, 14, 8179.	1.3	52
66	First principles nuclear magnetic resonance signatures of graphene oxide. Journal of Chemical Physics, 2010, 133, 034502.	1.2	51
67	Orbital Interaction Mechanisms of Conductance Enhancement and Rectification by Dithiocarboxylate Anchoring Group. Journal of Physical Chemistry B, 2006, 110, 19116-19120.	1.2	50
68	Paleomagnetic constraints on the paleolatitude of the Lhasa block during the Early Cretaceous: Implications for the onset of Indiaâ€“Asia collision and latitudinal shortening estimates across Tibet and stable Asia. Gondwana Research, 2017, 41, 352-372.	3.0	49
69	A first-principles study of NO adsorption and oxidation on Au(111) surface. Journal of Chemical Physics, 2008, 129, 134708.	1.2	48
70	Gas-phase dynamics in graphene growth by chemical vapour deposition. Physical Chemistry Chemical Physics, 2015, 17, 22832-22836.	1.3	48
71	Nanoimprinted circular grating distributed feedback dye laser. Applied Physics Letters, 2007, 91, .	1.5	47
72	Diamond as an inert substrate of graphene. Journal of Chemical Physics, 2013, 138, 054701.	1.2	46

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73	Bilayer Graphene Growth via a Penetration Mechanism. Journal of Physical Chemistry C, 2014, 118, 6201-6206.	1.5	44
74	Transition-Metal Diboride: A New Family of Two-Dimensional Materials Designed for Selective CO₂ Electroreduction. Journal of Physical Chemistry C, 2019, 123, 16294-16299.	1.5	43
75	Inorganic Electride:â€‰ Theoretical Study on Structural and Electronic Properties. Journal of the American Chemical Society, 2003, 125, 6050-6051.	6.6	41
76	Electride: from computational characterization to theoretical design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 430-440.	6.2	41
77	Two-Dimensional Stoichiometric Boron Oxides as a Versatile Platform for Electronic Structure Engineering. Journal of Physical Chemistry Letters, 2017, 8, 4347-4353.	2.1	41
78	Discriminating early stage AÎ²42 monomer structures using chirality-induced 2DIR spectroscopy in a simulation study. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 15687-15692.	3.3	40
79	Atomically thin semiconducting penta-PdP₂ and PdAs₂ with ultrahigh carrier mobility. Journal of Materials Chemistry C, 2018, 6, 9055-9059.	2.7	39
80	Rational Design of Two-dimensional Anode Materials: B₂S as a Strained Graphene. Journal of Physical Chemistry Letters, 2018, 9, 4852-4856.	2.1	38
81	Provenance analysis of Cretaceous peripheral foreland basin in central Tibet: Implications to precise timing on the initial Lhasa-Qiangtang collision. Tectonophysics, 2020, 775, 228311.	0.9	37
82	Efficient Direct Band Gap Photovoltaic Material Predicted Via Doping Double Perovskites Cs₂AgBiX₆ (X = Cl, Br). Journal of Physical Chemistry C, 2021, 125, 10868-10875.	1.5	37
83	First Principles Study on the Geometric and Electronic Structures of the FeO/Pt(111) Surface. Journal of Physical Chemistry C, 2009, 113, 8302-8305.	1.5	36
84	<scp>HONPAS</scp>: A linear scaling openâ€source solution for large system simulations. International Journal of Quantum Chemistry, 2015, 115, 647-655.	1.0	34
85	A density functional study on cationic AunCum+ clusters and their monocarbonyls. Physical Chemistry Chemical Physics, 2009, 11, 2329.	1.3	33
86	A wearable IoT aldehyde sensor for pediatric asthma research and management. Sensors and Actuators B: Chemical, 2019, 287, 584-594.	4.0	33
87	Finite element simulations of hydrodynamic trapping in microfluidic particle-trap array systems. Biomicrofluidics, 2013, 7, 54108.	1.2	32
88	First-principles study ofMgB2(0001) surfaces. Physical Review B, 2002, 65, .	1.1	31
89	Probing Electron Correlations in Molecules by Two-Dimensional Coherent Optical Spectroscopy. Journal of the American Chemical Society, 2008, 130, 3509-3515.	6.6	31
90	Structure of Blue Phosphorus Grown on Au(111) Surface Revisited. Journal of Physical Chemistry C, 2020, 124, 2024-2029.	1.5	31

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91	First-principles lattice dynamics ofNaCoO2. Physical Review B, 2004, 70, .	1.1	30
92	Optofluidic Distributed Feedback Dye Lasers. IEEE Journal of Selected Topics in Quantum Electronics, 2007, 13, 185-193.	1.9	30
93	Electronic Structures of Defective Boron Nitride Nanotubes under Transverse Electric Fields. Journal of Physical Chemistry C, 2008, 112, 8424-8428.	1.5	30
94	Elementary Process for CVD Graphene on Cu(110): Size-selective Carbon Clusters. Scientific Reports, 2014, 4, 4431.	1.6	30
95	Two-dimensional electronic correlation spectroscopy of the nÏ€âˆ— and Ï€Ï€âˆ— protein backbone transitions: A simulation study. Chemical Physics, 2007, 341, 29-36.	0.9	28
96	Optimization of microfluidic microsphere-trap arrays. Biomicrofluidics, 2013, 7, 14112.	1.2	28
97	The Nanoparticle Size Effect in Graphene Cutting: A â€œPacâ€Manâ€•Mechanism. Angewandte Chemie - International Edition, 2016, 55, 9918-9921.	7.2	28
98	Growth of boron nitride nanotubes from magnesium diboride catalysts. Nanoscale, 2018, 10, 13895-13901.	2.8	28
99	Effects of discrete energy levels on single-electron tunneling in coupled metal particles. Applied Physics Letters, 2003, 82, 3767-3769.	1.5	27
100	Density Functional Study of Nonlinear Optical Properties of Grossly Warped Nanographene C₈₀H₃₀. Journal of Physical Chemistry C, 2014, 118, 3313-3318.	1.5	27
101	Atomistic Simulations of Graphene Growth: From Kinetics to Mechanism. Accounts of Chemical Research, 2018, 51, 728-735.	7.6	27
102	Simulating Periodic Systems on a Quantum Computer Using Molecular Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 6904-6914.	2.3	27
103	3D/2D TMSs/TiO2 nanofibers heterojunctions for photodynamic-photothermal and oxidase-like synergistic antibacterial therapy co-driven by VIS and NIR biowindows. Composites Part B: Engineering, 2022, 230, 109498.	5.9	27
104	A first principles study on organic molecule encapsulated boron nitride nanotubes. Journal of Chemical Physics, 2008, 128, 164701.	1.2	26
105	Boron K4 crystal: a stable chiral three-dimensional sp2 network. Physical Chemistry Chemical Physics, 2010, 12, 12420.	1.3	25
106	Equation-of-Motion Theory to Calculate Accurate Band Structures with a Quantum Computer. Journal of Physical Chemistry Letters, 2021, 12, 8833-8840.	2.1	25
107	Implementation of screened hybrid density functional for periodic systems with numerical atomic orbitals: Basis function fitting and integral screening. Journal of Chemical Physics, 2011, 135, 034110.	1.2	24
108	Diffusion and desorption of oxygen atoms on graphene. Journal of Physics Condensed Matter, 2013, 25, 405301.	0.7	24

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109	Theoretical Insights into Li-Ion Transport in LiTa₂PO₈. Journal of Physical Chemistry C, 2019, 123, 19282-19287.	1.5	24
110	Paleomagnetism of Middle Triassic Lavas From Northern Qiangtang (Tibet): Constraints on the Closure of the Paleoâ€Tethys Ocean. Journal of Geophysical Research: Solid Earth, 2020, 125, e2019JB017804.	1.4	24
111	Emerging forward osmosis and membrane distillation for liquid food concentration: A review. Comprehensive Reviews in Food Science and Food Safety, 2021, 20, 1910-1936.	5.9	24
112	Oxygen adsorption on Zr(0001) surfaces: Density functional calculations and a multiple-layer adsorption model. Surface Science, 2008, 602, 2212-2216.	0.8	23
113	Linear scaling electronic structure calculations with numerical atomic basis set. International Reviews in Physical Chemistry, 2010, 29, 665-691.	0.9	23
114	Proposal of a general scheme to obtain room-temperature spin polarization in asymmetric antiferromagnetic semiconductors. Physical Review B, 2015, 92, .	1.1	23
115	An efficient adaptive variational quantum solver of the SchrÃ¶dinger equation based on reduced density matrices. Journal of Chemical Physics, 2021, 154, 244112.	1.2	23
116	Single-Molecule Imaging of Activated Nitrogen Adsorption on Individual Manganese Phthalocyanine. Nano Letters, 2015, 15, 3181-3188.	4.5	22
117	Microfluidics-enabled 96-well perfusion system for high-throughput tissue engineering and long-term all-optical electrophysiology. Lab on A Chip, 2020, 20, 4031-4042.	3.1	22
118	Methanol-Selective Oxidation Pathways on Au Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 17511-17520.	1.5	21
119	A Density Functional Study of the Nonlinear Optical Properties of Edgeâ€Functionalized Nonplanar Nanographenes. ChemPhysChem, 2015, 16, 2783-2788.	1.0	21
120	Low-Temperature Heterolytic Adsorption of H₂ on ZnO(101Ì…0) Surface. Journal of Physical Chemistry C, 2019, 123, 13283-13287.	1.5	21
121	Disorder and Suppression of Quantum Confinement Effects in Pd Nanoparticles. Physical Review Letters, 2003, 90, 246803.	2.9	20
122	Geometry and excitation energy fluctuations of NMA in aqueous solution with CHARMM, AMBER, OPLS, and GROMOS force fields: Implications for protein ultraviolet spectra simulation. Chemical Physics Letters, 2008, 452, 78-83.	1.2	20
123	Rectifying Effect in Polar Conjugated Molecular Junctions: A First-Principles Study. Journal of Nanoscience and Nanotechnology, 2009, 9, 774-778.	0.9	20
124	Distinct molecule adsorption behaviors on warped nanographene C80H30: A theoretical study. Carbon, 2016, 100, 428-434.	5.4	20
125	Implementation of Exact Exchange with Numerical Atomic Orbitals. Journal of Physical Chemistry A, 2010, 114, 1039-1043.	1.1	19
126	Density functional predictions of new silicon allotropes: Electronic properties and potential applications to Li-battery anode materials. Solid State Communications, 2011, 151, 1228-1230.	0.9	19

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127	Streamline based design guideline for deterministic microfluidic hydrodynamic single cell traps. Biomicrofluidics, 2015, 9, 024103.	1.2	19
128	Spinâ€“phonon coupling in NiO nanoparticle. Journal of Applied Physics, 2020, 128, .	1.1	19
129	Geometrical, electronic, and magnetic properties ofNa0.5CoO2from first principles. Physical Review B, 2005, 71, .	1.1	18
130	Adsorption and Diffusion of CO on Clean and CO₂-Precovered ZnO(101Ì…0). Journal of Physical Chemistry C, 2018, 122, 8919-8924.	1.5	18
131	A Discreet Wearable IoT Sensor for Continuous Transdermal Alcohol Monitoringâ€”Challenges and Opportunities. IEEE Sensors Journal, 2021, 21, 5322-5330.	2.4	18
132	Electronic structures of organic molecule encapsulated BN nanotubes under transverse electric field. Journal of Chemical Physics, 2008, 129, 024710.	1.2	17
133	Surface and size effects on the charge state of NV center in nanodiamonds. Computational and Theoretical Chemistry, 2013, 1021, 49-53.	1.1	17
134	Inorganic Electrides. Chemistry - A European Journal, 2004, 10, 1592-1596.	1.7	16
135	A Kinetic Pathway toward High-Density Ordered N Doping of Epitaxial Graphene on Cu(111) Using C₅NCl₅ Precursors. Journal of the American Chemical Society, 2017, 139, 7196-7202.	6.6	16
136	Theoretical Insights into the Thermodynamics and Kinetics of Graphene Growth on Copper Surfaces. Journal of Physical Chemistry C, 2020, 124, 16233-16247.	1.5	16
137	Optofluidic circular grating distributed feedback dye laser. Applied Physics Letters, 2009, 95, 031109.	1.5	15
138	Thickness-Dependent Adsorption of Melamine on Cu/Au(111) Films. Journal of Physical Chemistry C, 2017, 121, 7977-7984.	1.5	15
139	Configuration and Timing of Collision Between Arabia and Eurasia in the Zagros Collision Zone, Fars, Southern Iran. Tectonics, 2021, 40, e2021TC006762.	1.3	15
140	Detecting a Moleculeâ^'Surface Hybrid State by an Fe-Coated Tip with a Non-s-Like Orbital. Journal of Physical Chemistry C, 2008, 112, 15603-15606.	1.5	14
141	Electron Transport in Butane Molecular Wires with Different Anchoring Groups Containing N, S, and P: A First Principles Study. Journal of Physical Chemistry C, 2009, 113, 21911-21914.	1.5	14
142	A computational infrared spectroscopic study of graphene oxide. Journal of Chemical Physics, 2013, 139, 084704.	1.2	14
143	Electronic and transport properties of graphene with grain boundaries. RSC Advances, 2016, 6, 1090-1097.	1.7	14
144	Ion Conductivity Enhancement in Antiâ€Spinel Li₃OBr with Intrinsic Vacancies. Advanced Theory and Simulations, 2019, 2, 1800138.	1.3	14

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145	Reaction Mechanism and Strategy for Optimizing the Hydrogen Evolution Reaction on Single-Layer 1Tâ€² WSe₂ and WTe₂ Based on Grand Canonical Potential Kinetics. ACS Applied Materials & Interfaces, 2021, 13, 55611-55620.	4.0	14
146	Single molecule tunneling spectroscopy investigation of reversibly switched dipolar vanadyl phthalocyanine on graphite. Applied Physics Letters, 2014, 104, .	1.5	13
147	First-Principles Study of Molecular Clusters Formed by Nitric Acid and Ammonia. Journal of Physical Chemistry A, 2017, 121, 661-668.	1.1	13
148	A Cloud-Connected NO₂ and Ozone Sensor System for Personalized Pediatric Asthma Research and Management. IEEE Sensors Journal, 2020, 20, 15143-15153.	2.4	13
149	One-Dimensional Magnetic Order Stabilized in Edge-Reconstructed MoS₂ Nanoribbon via Bias Voltage. Journal of Physical Chemistry Letters, 2020, 11, 7531-7535.	2.1	13
150	Blue Phosphorus Growth on Different Noble Metal Surfaces: From a 2D Alloy Network to an Extended Monolayer. Journal of Physical Chemistry C, 2021, 125, 675-679.	1.5	13
151	Linear scaling calculation of maximally localized Wannier functions with atomic basis set. Journal of Chemical Physics, 2006, 124, 234108.	1.2	12
152	First-Principles Simulation of Amide and Aromatic Side Chain Ultraviolet Spectroscopy of a Cyclic Dipeptide. Journal of Physical Chemistry A, 2007, 111, 11579-11583.	1.1	12
153	Are Azafullerene Encapsulated Single-Walled Carbon Nanotubes n-Type Semiconductors?. Journal of Physical Chemistry C, 2011, 115, 12760-12762.	1.5	12
154	Paleomagnetic constraints on the Cenozoic kinematic evolution of the Pamir plateau from the Western Kunlun Shan foreland. Tectonophysics, 2013, 603, 257-271.	0.9	12
155	Reversible Tuning of Interfacial and Intramolecular Charge Transfer in Individual MnPc Molecules. Nano Letters, 2015, 15, 8091-8098.	4.5	12
156	Stimuli-Responsive Lysozyme Nanocapsule Engineered Microfiltration Membranes with a Dual-Function of Anti-Adhesion and Antibacteria for Biofouling Mitigation. ACS Applied Materials & Interfaces, 2021, 13, 32205-32216.	4.0	12
157	Schottky and Ohmic Contacts at Î±-Tellurene/2D Metal Interfaces. ACS Applied Electronic Materials, 2022, 4, 1082-1088.	2.0	12
158	Single-stranded DNA adsorption on chiral molecule coated Au surface: a molecular dynamics study. Physical Chemistry Chemical Physics, 2010, 12, 4431.	1.3	11
159	Molecular Mechanism and Solvation Effect of Supramolecular Catalysis in a Synthetic Cavitand Receptor with an Inwardly Directed Carboxylic Acid for Ring-Opening Cyclization of Epoxy Alcohols. ACS Catalysis, 2018, 8, 11910-11925.	5.5	11
160	Molecular Mechanisms and Atmospheric Implications of Criegee Intermediateâ€“Alcohol Chemistry in the Gas Phase and Aqueous Surface Environments. Journal of Physical Chemistry A, 2020, 124, 8585-8593.	1.1	11
161	A Cloud-Connected Multi-Lead Electrocardiogram (ECG) Sensor Ring. IEEE Sensors Journal, 2021, 21, 16340-16349.	2.4	11
162	Boosting ionic conductivity in antiperovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Li</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:m via defect engineering: Interstitial versus vacancy. Physical Review Materials, 2019, 3, .	3.9	11

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163	STM studies of single molecules: molecular orbital aspects. Chemical Communications, 2011, 47, 2747.	2.2	10
164	Simultaneous detection of multiple biological targets using optimized microfluidic microsphere-trap arrays. Journal of Micro/ Nanolithography, MEMS, and MOEMS, 2014, 13, 1.	1.0	10
165	The mobility and solvation structure of a hydroxyl radical in a water nanodroplet: a Bornâ€“Oppenheimer molecular dynamics study. Physical Chemistry Chemical Physics, 2021, 23, 14628-14635.	1.3	10
166	Quantum algorithms for electronic structures: basis sets and boundary conditions. Chemical Society Reviews, 2022, 51, 3263-3279.	18.7	10
167	First-principles calculations of conductance within a plane wave basis set via non-orthogonal Wannier-type atomic orbitals. Journal of Physics Condensed Matter, 2006, 18, 1347-1358.	0.7	9
168	Orientation-sensitive nonlinear growth of graphene: An epitaxial growth mechanism determined by geometry. Physical Review B, 2013, 88, .	1.1	9
169	Predictive design of intrinsic half-metallicity in zigzag tungsten dichalcogenide nanoribbons. Physical Review B, 2019, 100, .	1.1	9
170	Half-filled intermediate bands in doped inorganic perovskites for solar cells. Physical Chemistry Chemical Physics, 2020, 22, 23804-23809.	1.3	9
171	Intrinsic ultra-wide completely spin-polarized state realized in a new CrO₂ monolayer. Physical Chemistry Chemical Physics, 2020, 22, 17038-17041.	1.3	9
172	Experimental Realization of One-Dimensional Metal-Inorganic Chain: Goldâ€“Phosphorus Chain. , 2020, 2, 873-879.		9
173	Electrochemistry of Pâ€“C Bonds in Phosphorusâ€“Carbon Based Anode Materials. ACS Applied Materials & Interfaces, 2022, 14, 18506-18512.	4.0	9
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