

# Zhenyu Li

## List of Publications by Year in descending order

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201  
papers

11,904  
citations

22153

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102  
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202  
all docs

202  
docs citations

202  
times ranked

13399  
citing authors

#	ARTICLE	IF	CITATIONS
1	Half-Metallicity in Edge-Modified Zigzag Graphene Nanoribbons. <i>Journal of the American Chemical Society</i> , 2008, 130, 4224-4225.	13.7	640
2	Epitaxial Growth of Single Layer Blue Phosphorus: A New Phase of Two-Dimensional Phosphorus. <i>Nano Letters</i> , 2016, 16, 4903-4908.	9.1	609
3	Low-Temperature Growth of Graphene by Chemical Vapor Deposition Using Solid and Liquid Carbon Sources. <i>ACS Nano</i> , 2011, 5, 3385-3390.	14.6	353
4	Single mode optofluidic distributed feedback dye laser. <i>Optics Express</i> , 2006, 14, 696.	3.4	335
5	How Graphene Is Cut upon Oxidation?. <i>Journal of the American Chemical Society</i> , 2009, 131, 6320-6321.	13.7	323
6	First-Principles Thermodynamics of Graphene Growth on Cu Surfaces. <i>Journal of Physical Chemistry C</i> , 2011, 115, 17782-17787.	3.1	317
7	Will zigzag graphene nanoribbon turn to half metal under electric field?. <i>Applied Physics Letters</i> , 2007, 91, .	3.3	299
8	Obtaining Two-Dimensional Electron Gas in Free Space without Resorting to Electron Doping: An Electride Based Design. <i>Journal of the American Chemical Society</i> , 2014, 136, 13313-13318.	13.7	280
9	Bipolar magnetic semiconductors: a new class of spintronics materials. <i>Nanoscale</i> , 2012, 4, 5680.	5.6	241
10	Proposed Photosynthesis Method for Producing Hydrogen from Dissociated Water Molecules Using Incident Near-Infrared Light. <i>Physical Review Letters</i> , 2014, 112, 018301.	7.8	237
11	A first-principles study of gas adsorption on germanene. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22495-22498.	2.8	232
12	Electronic structures of SiC nanoribbons. <i>Journal of Chemical Physics</i> , 2008, 129, 174114.	3.0	222
13	Silicene as a highly sensitive molecule sensor for NH <sub>3</sub> , NO and NO <sub>2</sub> . <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6957.	2.8	221
14	Oxygen molecule dissociation on carbon nanostructures with different types of nitrogen doping. <i>Nanoscale</i> , 2012, 4, 1184-1189.	5.6	220
15	A multi-color fast-switching microfluidic droplet dye laser. <i>Lab on A Chip</i> , 2009, 9, 2767.	6.0	177
16	Adsorption energies of molecular oxygen on Au clusters. <i>Journal of Chemical Physics</i> , 2004, 120, 9594-9600.	3.0	159
17	Mo <sub>2</sub> C nanoparticles embedded within bacterial cellulose-derived 3D N-doped carbon nanofiber networks for efficient hydrogen evolution. <i>NPG Asia Materials</i> , 2016, 8, e288-e288.	7.9	153
18	Site-specific photocatalytic splitting of methanol on TiO <sub>2</sub> (110). <i>Chemical Science</i> , 2010, 1, 575.	7.4	150

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19	Optofluidic dye lasers. <i>Microfluidics and Nanofluidics</i> , 2008, 4, 145-158.	2.2	143
20	Remarkable chemical adsorption of manganese-doped titanate for direct carbon dioxide electrolysis. <i>Journal of Materials Chemistry A</i> , 2014, 2, 6904-6915.	10.3	137
21	Half-metallicity in hybrid BCN nanoribbons. <i>Journal of Chemical Physics</i> , 2008, 129, 084712.	3.0	133
22	Electronic Structure Engineering via On-Plane Chemical Functionalization: A Comparison Study on Two-Dimensional Polysilane and Graphane. <i>Journal of Physical Chemistry C</i> , 2009, 113, 16741-16746.	3.1	133
23	Mechanically tunable optofluidic distributed feedback dye laser. <i>Optics Express</i> , 2006, 14, 10494.	3.4	128
24	Porous silicene as a hydrogen purification membrane. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5753.	2.8	127
25	Pt Single Atoms Embedded in the Surface of Ni Nanocrystals as Highly Active Catalysts for Selective Hydrogenation of Nitro Compounds. <i>Nano Letters</i> , 2018, 18, 3785-3791.	9.1	127
26	Electron-phonon coupling in a boron-doped diamond superconductor. <i>Physical Review B</i> , 2004, 70, .	3.2	126
27	Paleomagnetic constraints on the Mesozoic drift of the Lhasa terrane (Tibet) from Gondwana to Eurasia. <i>Geology</i> , 2016, 44, 727-730.	4.4	118
28	Growth of Quasi-Free-Standing Single-Layer Blue Phosphorus on Tellurium Monolayer Functionalized Au(111). <i>ACS Nano</i> , 2017, 11, 4943-4949.	14.6	109
29	Single-Molecule Chemistry of Metal Phthalocyanine on Noble Metal Surfaces. <i>Accounts of Chemical Research</i> , 2010, 43, 954-962.	15.6	105
30	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. <i>Journal of Physical Chemistry C</i> , 2012, 116, 3142-3146.	3.1	103
31	Late Triassic paleolatitude of the Qiangtang block: Implications for the closure of the Paleo-Tethys Ocean. <i>Earth and Planetary Science Letters</i> , 2015, 424, 69-83.	4.4	98
32	Electronic and optical properties of graphene and graphitic ZnO nanocomposite structures. <i>Journal of Chemical Physics</i> , 2013, 138, 124706.	3.0	97
33	Helium separation via porous silicene based ultimate membrane. <i>Nanoscale</i> , 2013, 5, 9062.	5.6	96
34	Aerobic Oxidation of Cyclohexane on Catalysts Based on Twinned and Single-Crystal Au <sub>75</sub> Pd <sub>25</sub> Bimetallic Nanocrystals. <i>Nano Letters</i> , 2015, 15, 2875-2880.	9.1	92
35	Structure of Graphene Oxide: Thermodynamics versus Kinetics. <i>Journal of Physical Chemistry C</i> , 2011, 115, 11991-11995.	3.1	91
36	The early Eocene rise of the Gonjo Basin, SE Tibet: From low desert to high forest. <i>Earth and Planetary Science Letters</i> , 2020, 543, 116312.	4.4	91

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37	Precursor Triggering Synthesis of Self-Coupled Sulfide Polymorphs with Enhanced Photoelectrochemical Properties. <i>Journal of the American Chemical Society</i> , 2016, 138, 12913-12919.	13.7	90
38	Oxidation states of graphene: Insights from computational spectroscopy. <i>Journal of Chemical Physics</i> , 2009, 131, 244505.	3.0	88
39	Lattice Mismatch Induced Nonlinear Growth of Graphene. <i>Journal of the American Chemical Society</i> , 2012, 134, 6045-6051.	13.7	88
40	Structural, electronic, and optical properties of hybrid silicene and graphene nanocomposite. <i>Journal of Chemical Physics</i> , 2013, 139, 154704.	3.0	84
41	Flexible packaging of solid-state integrated circuit chips with elastomeric microfluidics. <i>Scientific Reports</i> , 2013, 3, .	3.3	83
42	Single Faceted Two-Dimensional Mo <sub>2</sub> C Electrocatalyst for Highly Efficient Nitrogen Fixation. <i>ACS Catalysis</i> , 2020, 10, 7864-7870.	11.2	80
43	The rise and demise of the Paleogene Central Tibetan Valley. <i>Science Advances</i> , 2022, 8, eabj0944.	10.3	80
44	Theoretical study of nitric oxide adsorption on Au clusters. <i>Journal of Chemical Physics</i> , 2004, 121, 2558.	3.0	78
45	Dithiocarbamate Anchoring in Molecular Wire Junctions: A First Principles Study. <i>Journal of Physical Chemistry B</i> , 2006, 110, 9893-9898.	2.6	78
46	Ratio-Controlled Synthesis of CuNi Octahedra and Nanocubes with Enhanced Catalytic Activity. <i>Journal of the American Chemical Society</i> , 2015, 137, 14027-14030.	13.7	75
47	Contrasting Structural Reconstructions, Electronic Properties, and Magnetic Orderings along Different Edges of Zigzag Transition Metal Dichalcogenide Nanoribbons. <i>Nano Letters</i> , 2017, 17, 1097-1101.	9.1	75
48	Nature of well-defined conductance of amine-anchored molecular junctions: Density functional calculations. <i>Physical Review B</i> , 2007, 76, .	3.2	74
49	Mechanisms of Graphene Growth on Metal Surfaces: Theoretical Perspectives. <i>Small</i> , 2014, 10, 2136-2150.	10.0	73
50	Carbon Dimers as the Dominant Feeding Species in Epitaxial Growth and Morphological Phase Transition of Graphene on Different Cu Substrates. <i>Physical Review Letters</i> , 2015, 114, 216102.	7.8	73
51	Communication: Coalescence of carbon atoms on Cu (111) surface: Emergence of a stable bridging-metal structure motif. <i>Journal of Chemical Physics</i> , 2010, 133, 071101.	3.0	72
52	MAGNETISM IN GRAPHENE SYSTEMS. <i>Nano</i> , 2008, 03, 433-442.	1.0	70
53	Graphene Thickness Control via Gas-Phase Dynamics in Chemical Vapor Deposition. <i>Journal of Physical Chemistry C</i> , 2012, 116, 10557-10562.	3.1	70
54	Is Mayenite without Clathrated Oxygen an Inorganic Electride?. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 6479-6482.	13.8	68

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55	A first-principles prediction of two-dimensional superconductivity in pristine B2C single layers. <i>Nanoscale</i> , 2012, 4, 3032.	5.6	67
56	An early bird from Gondwana: Paleomagnetism of Lower Permian lavas from northern Qiangtang (Tibet) and the geography of the Paleo-Tethys. <i>Earth and Planetary Science Letters</i> , 2017, 475, 119-133.	4.4	67
57	Optofluidic evanescent dye laser based on a distributed feedback circular grating. <i>Applied Physics Letters</i> , 2009, 94, 161110.	3.3	66
58	Effects of nano- and microplastics on kidney: Physicochemical properties, bioaccumulation, oxidative stress and immunoreaction. <i>Chemosphere</i> , 2022, 288, 132631.	8.2	66
59	Descriptor-Based Design Principle for Two-Dimensional Single-Atom Catalysts: Carbon Dioxide Electroreduction. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3481-3487.	4.6	65
60	Dominant Kinetic Pathways of Graphene Growth in Chemical Vapor Deposition: The Role of Hydrogen. <i>Journal of Physical Chemistry C</i> , 2017, 121, 25949-25955.	3.1	61
61	Low-order distributed feedback optofluidic dye laser with reduced threshold. <i>Applied Physics Letters</i> , 2009, 94, .	3.3	56
62	Hydrogenated bilayer wurtzite SiC nanofilms: a two-dimensional bipolar magnetic semiconductor material. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 497-503.	2.8	55
63	Antibody Quantum Dot Conjugates Developed via Copper-Free Click Chemistry for Rapid Analysis of Biological Samples Using a Microfluidic Microsphere Array System. <i>Bioconjugate Chemistry</i> , 2014, 25, 1272-1281.	3.6	55
64	A smartphone controlled handheld microfluidic liquid handling system. <i>Lab on A Chip</i> , 2014, 14, 4085-4092.	6.0	54
65	Diamondization of chemically functionalized graphene and grapheneâ€“BN bilayers. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8179.	2.8	52
66	First principles nuclear magnetic resonance signatures of graphene oxide. <i>Journal of Chemical Physics</i> , 2010, 133, 034502.	3.0	51
67	Orbital Interaction Mechanisms of Conductance Enhancement and Rectification by Dithiocarboxylate Anchoring Group. <i>Journal of Physical Chemistry B</i> , 2006, 110, 19116-19120.	2.6	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. <i>Gondwana Research</i> , 2017, 41, 352-372.	6.0	49
69	A first-principles study of NO adsorption and oxidation on Au(111) surface. <i>Journal of Chemical Physics</i> , 2008, 129, 134708.	3.0	48
70	Gas-phase dynamics in graphene growth by chemical vapour deposition. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22832-22836.	2.8	48
71	Nanoimprinted circular grating distributed feedback dye laser. <i>Applied Physics Letters</i> , 2007, 91, .	3.3	47
72	Diamond as an inert substrate of graphene. <i>Journal of Chemical Physics</i> , 2013, 138, 054701.	3.0	46

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73	Bilayer Graphene Growth via a Penetration Mechanism. <i>Journal of Physical Chemistry C</i> , 2014, 118, 6201-6206.	3.1	44
74	Transition-Metal Diboride: A New Family of Two-Dimensional Materials Designed for Selective CO <sub>2</sub> Electroreduction. <i>Journal of Physical Chemistry C</i> , 2019, 123, 16294-16299.	3.1	43
75	Inorganic Electride: A Theoretical Study on Structural and Electronic Properties. <i>Journal of the American Chemical Society</i> , 2003, 125, 6050-6051.	13.7	41
76	Electride: from computational characterization to theoretical design. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016, 6, 430-440.	14.6	41
77	Two-Dimensional Stoichiometric Boron Oxides as a Versatile Platform for Electronic Structure Engineering. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4347-4353.	4.6	41
78	Discriminating early stage Al <sup>2+</sup> monomer structures using chirality-induced 2DIR spectroscopy in a simulation study. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 15687-15692.	7.1	40
79	Atomically thin semiconducting penta-PdP <sub>2</sub> and PdAs <sub>2</sub> with ultrahigh carrier mobility. <i>Journal of Materials Chemistry C</i> , 2018, 6, 9055-9059.	5.5	39
80	Rational Design of Two-dimensional Anode Materials: B <sub>2</sub> S as a Strained Graphene. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4852-4856.	4.6	38
81	Provenance analysis of Cretaceous peripheral foreland basin in central Tibet: Implications to precise timing on the initial Lhasa-Qiangtang collision. <i>Tectonophysics</i> , 2020, 775, 228311.	2.2	37
82	Efficient Direct Band Gap Photovoltaic Material Predicted via Doping Double Perovskites Cs <sub>2</sub> AgBiX <sub>6</sub> (X = Cl, Br). <i>Journal of Physical Chemistry C</i> , 2021, 125, 10868-10875.	3.1	37
83	First Principles Study on the Geometric and Electronic Structures of the FeO/Pt(111) Surface. <i>Journal of Physical Chemistry C</i> , 2009, 113, 8302-8305.	3.1	36
84	HONPAS: A linear scaling open-source solution for large system simulations. <i>International Journal of Quantum Chemistry</i> , 2015, 115, 647-655.	2.0	34
85	A density functional study on cationic Au <sub>n</sub> Cu <sub>m</sub> <sup>+</sup> clusters and their monocarbonyls. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 2329.	2.8	33
86	A wearable IoT aldehyde sensor for pediatric asthma research and management. <i>Sensors and Actuators B: Chemical</i> , 2019, 287, 584-594.	7.8	33
87	Finite element simulations of hydrodynamic trapping in microfluidic particle-trap array systems. <i>Biomicrofluidics</i> , 2013, 7, 54108.	2.4	32
88	First-principles study of MgB <sub>2</sub> (0001) surfaces. <i>Physical Review B</i> , 2002, 65, .	3.2	31
89	Probing Electron Correlations in Molecules by Two-Dimensional Coherent Optical Spectroscopy. <i>Journal of the American Chemical Society</i> , 2008, 130, 3509-3515.	13.7	31
90	Structure of Blue Phosphorus Grown on Au(111) Surface Revisited. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2024-2029.	3.1	31

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91	First-principles lattice dynamics of NaCoO <sub>2</sub> . <i>Physical Review B</i> , 2004, 70, .	3.2	30
92	Optofluidic Distributed Feedback Dye Lasers. <i>IEEE Journal of Selected Topics in Quantum Electronics</i> , 2007, 13, 185-193.	2.9	30
93	Electronic Structures of Defective Boron Nitride Nanotubes under Transverse Electric Fields. <i>Journal of Physical Chemistry C</i> , 2008, 112, 8424-8428.	3.1	30
94	Elementary Process for CVD Graphene on Cu(110): Size-selective Carbon Clusters. <i>Scientific Reports</i> , 2014, 4, 4431.	3.3	30
95	Two-dimensional electronic correlation spectroscopy of the $\alpha$ - and $\beta$ -protein backbone transitions: A simulation study. <i>Chemical Physics</i> , 2007, 341, 29-36.	1.9	28
96	Optimization of microfluidic microsphere-trap arrays. <i>Biomicrofluidics</i> , 2013, 7, 14112.	2.4	28
97	The Nanoparticle Size Effect in Graphene Cutting: A Mechanism. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9918-9921.	13.8	28
98	Growth of boron nitride nanotubes from magnesium diboride catalysts. <i>Nanoscale</i> , 2018, 10, 13895-13901.	5.6	28
99	Effects of discrete energy levels on single-electron tunneling in coupled metal particles. <i>Applied Physics Letters</i> , 2003, 82, 3767-3769.	3.3	27
100	Density Functional Study of Nonlinear Optical Properties of Grossly Warped Nanographene C <sub>80</sub> H <sub>30</sub> . <i>Journal of Physical Chemistry C</i> , 2014, 118, 3313-3318.	3.1	27
101	Atomistic Simulations of Graphene Growth: From Kinetics to Mechanism. <i>Accounts of Chemical Research</i> , 2018, 51, 728-735.	15.6	27
102	Simulating Periodic Systems on a Quantum Computer Using Molecular Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6904-6914.	5.3	27
103	3D/2D TMSs/TiO <sub>2</sub> nanofibers heterojunctions for photodynamic-photothermal and oxidase-like synergistic antibacterial therapy co-driven by VIS and NIR biowindows. <i>Composites Part B: Engineering</i> , 2022, 230, 109498.	12.0	27
104	A first principles study on organic molecule encapsulated boron nitride nanotubes. <i>Journal of Chemical Physics</i> , 2008, 128, 164701.	3.0	26
105	Boron K <sub>4</sub> crystal: a stable chiral three-dimensional sp <sup>2</sup> network. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12420.	2.8	25
106	Equation-of-Motion Theory to Calculate Accurate Band Structures with a Quantum Computer. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8833-8840.	4.6	25
107	Implementation of screened hybrid density functional for periodic systems with numerical atomic orbitals: Basis function fitting and integral screening. <i>Journal of Chemical Physics</i> , 2011, 135, 034110.	3.0	24
108	Diffusion and desorption of oxygen atoms on graphene. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 405301.	1.8	24

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109	Theoretical Insights into Li-Ion Transport in $\text{LiTa}_2\text{PO}_8$ . <i>Journal of Physical Chemistry C</i> , 2019, 123, 19282-19287.	3.1	24
110	Paleomagnetism of Middle Triassic Lavas From Northern Qiangtang (Tibet): Constraints on the Closure of the Paleotethys Ocean. <i>Journal of Geophysical Research: Solid Earth</i> , 2020, 125, e2019JB017804.	3.4	24
111	Emerging forward osmosis and membrane distillation for liquid food concentration: A review. <i>Comprehensive Reviews in Food Science and Food Safety</i> , 2021, 20, 1910-1936.	11.7	24
112	Oxygen adsorption on Zr(0001) surfaces: Density functional calculations and a multiple-layer adsorption model. <i>Surface Science</i> , 2008, 602, 2212-2216.	1.9	23
113	Linear scaling electronic structure calculations with numerical atomic basis set. <i>International Reviews in Physical Chemistry</i> , 2010, 29, 665-691.	2.3	23
114	Proposal of a general scheme to obtain room-temperature spin polarization in asymmetric antiferromagnetic semiconductors. <i>Physical Review B</i> , 2015, 92, .	3.2	23
115	An efficient adaptive variational quantum solver of the Schrödinger equation based on reduced density matrices. <i>Journal of Chemical Physics</i> , 2021, 154, 244112.	3.0	23
116	Single-Molecule Imaging of Activated Nitrogen Adsorption on Individual Manganese Phthalocyanine. <i>Nano Letters</i> , 2015, 15, 3181-3188.	9.1	22
117	Microfluidics-enabled 96-well perfusion system for high-throughput tissue engineering and long-term all-optical electrophysiology. <i>Lab on A Chip</i> , 2020, 20, 4031-4042.	6.0	22
118	Methanol-Selective Oxidation Pathways on Au Surfaces: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2014, 118, 17511-17520.	3.1	21
119	A Density Functional Study of the Nonlinear Optical Properties of Edge-Functionalized Nonplanar Nanographenes. <i>ChemPhysChem</i> , 2015, 16, 2783-2788.	2.1	21
120	Low-Temperature Heterolytic Adsorption of $\text{H}_2$ on $\text{ZnO}(10\bar{1}1\cdot\cdot0)$ Surface. <i>Journal of Physical Chemistry C</i> , 2019, 123, 13283-13287.	3.1	21
121	Disorder and Suppression of Quantum Confinement Effects in Pd Nanoparticles. <i>Physical Review Letters</i> , 2003, 90, 246803.	7.8	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. <i>Chemical Physics Letters</i> , 2008, 452, 78-83.	2.6	20
123	Rectifying Effect in Polar Conjugated Molecular Junctions: A First-Principles Study. <i>Journal of Nanoscience and Nanotechnology</i> , 2009, 9, 774-778.	0.9	20
124	Distinct molecule adsorption behaviors on warped nanographene $\text{C}_{80}\text{H}_{30}$ : A theoretical study. <i>Carbon</i> , 2016, 100, 428-434.	10.3	20
125	Implementation of Exact Exchange with Numerical Atomic Orbitals. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1039-1043.	2.5	19
126	Density functional predictions of new silicon allotropes: Electronic properties and potential applications to Li-battery anode materials. <i>Solid State Communications</i> , 2011, 151, 1228-1230.	1.9	19



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127	Streamline based design guideline for deterministic microfluidic hydrodynamic single cell traps. <i>Biomicrofluidics</i> , 2015, 9, 024103.	2.4	19
128	Spinâ€“phonon coupling in NiO nanoparticle. <i>Journal of Applied Physics</i> , 2020, 128, .	2.5	19
129	Geometrical, electronic, and magnetic properties of Na <sub>0.5</sub> CoO <sub>2</sub> from first principles. <i>Physical Review B</i> , 2005, 71, .	3.2	18
130	Adsorption and Diffusion of CO on Clean and CO <sub>2</sub> -Precovered ZnO(101̄1̄0). <i>Journal of Physical Chemistry C</i> , 2018, 122, 8919-8924.	3.1	18
131	A Discreet Wearable IoT Sensor for Continuous Transdermal Alcohol Monitoringâ€“Challenges and Opportunities. <i>IEEE Sensors Journal</i> , 2021, 21, 5322-5330.	4.7	18
132	Electronic structures of organic molecule encapsulated BN nanotubes under transverse electric field. <i>Journal of Chemical Physics</i> , 2008, 129, 024710.	3.0	17
133	Surface and size effects on the charge state of NV center in nanodiamonds. <i>Computational and Theoretical Chemistry</i> , 2013, 1021, 49-53.	2.5	17
134	Inorganic Electrdes. <i>Chemistry - A European Journal</i> , 2004, 10, 1592-1596.	3.3	16
135	A Kinetic Pathway toward High-Density Ordered N Doping of Epitaxial Graphene on Cu(111) Using C <sub>5</sub> NCl <sub>5</sub> Precursors. <i>Journal of the American Chemical Society</i> , 2017, 139, 7196-7202.	13.7	16
136	Theoretical Insights into the Thermodynamics and Kinetics of Graphene Growth on Copper Surfaces. <i>Journal of Physical Chemistry C</i> , 2020, 124, 16233-16247.	3.1	16
137	Optofluidic circular grating distributed feedback dye laser. <i>Applied Physics Letters</i> , 2009, 95, 031109.	3.3	15
138	Thickness-Dependent Adsorption of Melamine on Cu/Au(111) Films. <i>Journal of Physical Chemistry C</i> , 2017, 121, 7977-7984.	3.1	15
139	Configuration and Timing of Collision Between Arabia and Eurasia in the Zagros Collision Zone, Fars, Southern Iran. <i>Tectonics</i> , 2021, 40, e2021TC006762.	2.8	15
140	Detecting a Moleculeâ€™s Surface Hybrid State by an Fe-Coated Tip with a Non-s-Like Orbital. <i>Journal of Physical Chemistry C</i> , 2008, 112, 15603-15606.	3.1	14
141	Electron Transport in Butane Molecular Wires with Different Anchoring Groups Containing N, S, and P: A First Principles Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21911-21914.	3.1	14
142	A computational infrared spectroscopic study of graphene oxide. <i>Journal of Chemical Physics</i> , 2013, 139, 084704.	3.0	14
143	Electronic and transport properties of graphene with grain boundaries. <i>RSC Advances</i> , 2016, 6, 1090-1097.	3.6	14
144	Ion Conductivity Enhancement in Antiâ€“spinel Li <sub>3</sub> OBr with Intrinsic Vacancies. <i>Advanced Theory and Simulations</i> , 2019, 2, 1800138.	2.8	14

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145	Reaction Mechanism and Strategy for Optimizing the Hydrogen Evolution Reaction on Single-Layer 1Tâ€² WSe <sub>2</sub> and WTe <sub>2</sub> Based on Grand Canonical Potential Kinetics. ACS Applied Materials & Interfaces, 2021, 13, 55611-55620.	8.0	14
146	Single molecule tunneling spectroscopy investigation of reversibly switched dipolar vanadyl phthalocyanine on graphite. Applied Physics Letters, 2014, 104, .	3.3	13
147	First-Principles Study of Molecular Clusters Formed by Nitric Acid and Ammonia. Journal of Physical Chemistry A, 2017, 121, 661-668.	2.5	13
148	A Cloud-Connected NO <sub>2</sub> and Ozone Sensor System for Personalized Pediatric Asthma Research and Management. IEEE Sensors Journal, 2020, 20, 15143-15153.	4.7	13
149	One-Dimensional Magnetic Order Stabilized in Edge-Reconstructed MoS <sub>2</sub> Nanoribbon via Bias Voltage. Journal of Physical Chemistry Letters, 2020, 11, 7531-7535.	4.6	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.	3.1	13
151	Linear scaling calculation of maximally localized Wannier functions with atomic basis set. Journal of Chemical Physics, 2006, 124, 234108.	3.0	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.	2.5	12
153	Are Azafullerene Encapsulated Single-Walled Carbon Nanotubes n-Type Semiconductors?. Journal of Physical Chemistry C, 2011, 115, 12760-12762.	3.1	12
154	Paleomagnetic constraints on the Cenozoic kinematic evolution of the Pamir plateau from the Western Kunlun Shan foreland. Tectonophysics, 2013, 603, 257-271.	2.2	12
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