

Zhenyu Li

List of Publications by Year in descending order

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201
papers

11,904
citations

22153

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30922

102
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202
all docs

202
docs citations

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times ranked

13399
citing authors

#	ARTICLE	IF	CITATIONS
1	Effects of nano- and microplastics on kidney: Physicochemical properties, bioaccumulation, oxidative stress and immunoreaction. <i>Chemosphere</i> , 2022, 288, 132631.	8.2	66
2	3D/2D TMSs/TiO ₂ 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
3	Understanding High-Temperature Chemical Reactions on Metal Surfaces: A Case Study on Equilibrium Concentration and Diffusivity of C _x H _y on a Cu(111) Surface. <i>Jacs Au</i> , 2022, 2, 443-452.	7.9	8
4	Personal NO ₂ sensor demonstrates feasibility of in-home exposure measurements for pediatric asthma research and management. <i>Journal of Exposure Science and Environmental Epidemiology</i> , 2022, 32, 312-319.	3.9	6
5	Unveiling the Atomic Structure and Growth Dynamics of One-Dimensional Water on ZnO(10 ¹⁰). <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1554-1562.	4.6	4
6	Quantum algorithms for electronic structures: basis sets and boundary conditions. <i>Chemical Society Reviews</i> , 2022, 51, 3263-3279.	38.1	10
7	The Important Role of Optical Absorption in Determining the Efficiency of Intermediate Band Solar Cells and a Design Principle for Perovskite Doping. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2012-2018.	4.6	7
8	Schottky and Ohmic Contacts at $\hat{\pm}$ -Tellurene/2D Metal Interfaces. <i>ACS Applied Electronic Materials</i> , 2022, 4, 1082-1088.	4.3	12
9	Electrochemistry of P-C Bonds in Phosphorus-Carbon Based Anode Materials. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 18506-18512.	8.0	9
10	The rise and demise of the Paleogene Central Tibetan Valley. <i>Science Advances</i> , 2022, 8, eabj0944.	10.3	80
11	New Paleomagnetic Constraints on the Early Cretaceous Paleolatitude of the Lhasa Terrane (Tibet). <i>Frontiers in Earth Science</i> , 2022, 10, .	1.8	2
12	Reducing Circuit Depth in Adaptive Variational Quantum Algorithms via Effective Hamiltonian Theories. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4795-4805.	5.3	7
13	A Discreet Wearable IoT Sensor for Continuous Transdermal Alcohol Monitoring—Challenges and Opportunities. <i>IEEE Sensors Journal</i> , 2021, 21, 5322-5330.	4.7	18
14	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
15	Atom by Atom Condensation of Sn Single Clusters within Gold-Phosphorus Metal-Inorganic Pore Networks. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 745-751.	4.6	8
16	The mobility and solvation structure of a hydroxyl radical in a water nanodroplet: a Born-Oppenheimer molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 14628-14635.	2.8	10
17	Efficient Direct Band Gap Photovoltaic Material Predicted via Doping Double Perovskites Cs ₂ AgBiX ₆ (X = Cl, Br). <i>Journal of Physical Chemistry C</i> , 2021, 125, 10868-10875.	3.1	37
18	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

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19	Stimuli-Responsive Lysozyme Nanocapsule Engineered Microfiltration Membranes with a Dual-Function of Anti-Adhesion and Antibacteria for Biofouling Mitigation. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 32205-32216.	8.0	12
20	A Cloud-Connected Multi-Lead Electrocardiogram (ECG) Sensor Ring. <i>IEEE Sensors Journal</i> , 2021, 21, 16340-16349.	4.7	11
21	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
22	Intrinsic Descriptors for Coordination Environment and Synergistic Effects of Metal and Environment in Single-Atom-Catalyzed Carbon Dioxide Electroreduction. <i>Journal of Physical Chemistry C</i> , 2021, 125, 18180-18186.	3.1	6
23	Reaction between a NO ₂ Dimer and Dissolved SO ₂ : A New Mechanism for ONSO ₃ Formation and its Fate in Aerosol. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8468-8475.	2.5	2
24	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
25	Blue Phosphorus Growth on Different Noble Metal Surfaces: From a 2D Alloy Network to an Extended Monolayer. <i>Journal of Physical Chemistry C</i> , 2021, 125, 675-679.	3.1	13
26	Reaction Mechanism and Strategy for Optimizing the Hydrogen Evolution Reaction on Single-Layer 1Tâ€² WSe ₂ and WTe ₂ Based on Grand Canonical Potential Kinetics. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 55611-55620.	8.0	14
27	Single Molecular Reaction of Water on a ZnO Surface. <i>Nano Letters</i> , 2021, 21, 9567-9572.	9.1	7
28	Structure of Blue Phosphorus Grown on Au(111) Surface Revisited. <i>Journal of Physical Chemistry C</i> , 2020, 124, 2024-2029.	3.1	31
29	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
30	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
31	Spinâ€“phonon coupling in NiO nanoparticle. <i>Journal of Applied Physics</i> , 2020, 128, .	2.5	19
32	Half-filled intermediate bands in doped inorganic perovskites for solar cells. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23804-23809.	2.8	9
33	Intrinsic ultra-wide completely spin-polarized state realized in a new CrO ₂ monolayer. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17038-17041.	2.8	9
34	A Cloud-Connected NO ₂ and Ozone Sensor System for Personalized Pediatric Asthma Research and Management. <i>IEEE Sensors Journal</i> , 2020, 20, 15143-15153.	4.7	13
35	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
36	Molecular Mechanisms and Atmospheric Implications of Criegee Intermediateâ€“Alcohol Chemistry in the Gas Phase and Aqueous Surface Environments. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8585-8593.	2.5	11

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37	On-Surface Synthesis of Nitrogen-Substituted Gold-Phosphorus Porous Network. Chemistry of Materials, 2020, 32, 8561-8566.	6.7	3
38	One-Dimensional Magnetic Order Stabilized in Edge-Reconstructed MoS ₂ Nanoribbon via Bias Voltage. Journal of Physical Chemistry Letters, 2020, 11, 7531-7535.	4.6	13
39	Intrinsic ferromagnetic semiconductivity realized in a new MoS ₂ monolayer. Physical Chemistry Chemical Physics, 2020, 22, 13363-13367.	2.8	2
40	Experimental Realization of One-Dimensional Metal-Inorganic Chain: Gold-Phosphorus Chain. , 2020, 2, 873-879.		9
41	Theoretical Insights into the Thermodynamics and Kinetics of Graphene Growth on Copper Surfaces. Journal of Physical Chemistry C, 2020, 124, 16233-16247.	3.1	16
42	Single Faceted Two-Dimensional Mo ₂ C Electrocatalyst for Highly Efficient Nitrogen Fixation. ACS Catalysis, 2020, 10, 7864-7870.	11.2	80
43	Platinum doped alkali earth metal oxides as a qubit candidate. Computational Materials Science, 2020, 181, 109754.	3.0	1
44	Paleomagnetism of Middle Triassic Lavas From Northern Qiangtang (Tibet): Constraints on the Closure of the Paleotethys Ocean. Journal of Geophysical Research: Solid Earth, 2020, 125, e2019JB017804.	3.4	24
45	Descriptor-Based Design Principle for Two-Dimensional Single-Atom Catalysts: Carbon Dioxide Electroreduction. Journal of Physical Chemistry Letters, 2020, 11, 3481-3487.	4.6	65
46	The early Eocene rise of the Gonjo Basin, SE Tibet: From low desert to high forest. Earth and Planetary Science Letters, 2020, 543, 116312.	4.4	91
47	Theoretical Insights into Li-Ion Transport in LiTa ₂ PO ₈ . Journal of Physical Chemistry C, 2019, 123, 19282-19287.	3.1	24
48	Ion Conductivity Enhancement in Anti-Spinel Li ₃ OBr with Intrinsic Vacancies. Advanced Theory and Simulations, 2019, 2, 1800138.	2.8	14
49	Transition-Metal Diboride: A New Family of Two-Dimensional Materials Designed for Selective CO ₂ Electroreduction. Journal of Physical Chemistry C, 2019, 123, 16294-16299.	3.1	43
50	Low-Temperature Heterolytic Adsorption of H ₂ on ZnO(101̄...0) Surface. Journal of Physical Chemistry C, 2019, 123, 13283-13287.	3.1	21
51	A wearable IoT aldehyde sensor for pediatric asthma research and management. Sensors and Actuators B: Chemical, 2019, 287, 584-594.	7.8	33
52	Predictive design of intrinsic half-metallicity in zigzag tungsten dichalcogenide nanoribbons. Physical Review B, 2019, 100, .	3.2	9
53	Molecular Dynamics Simulations of Noble Gas Fractionation during Diffusion through Silica Nanopores. ACS Earth and Space Chemistry, 2019, 3, 62-69.	2.7	1
54	Boosting ionic conductivity in antiperovskite $\text{Li}_{1-x}\text{M}_x\text{Ta}_{1-x}\text{Nb}_x\text{O}_{10}$ via defect engineering: Interstitial versus vacancy. Physical Review Materials, 2019, 3, .	3.4	11

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55	Atomistic Simulations of Graphene Growth: From Kinetics to Mechanism. <i>Accounts of Chemical Research</i> , 2018, 51, 728-735.	15.6	27
56	Adsorption and Diffusion of CO on Clean and CO ₂ -Precovered ZnO(101̄1̄0). <i>Journal of Physical Chemistry C</i> , 2018, 122, 8919-8924.	3.1	18
57	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. <i>ACS Catalysis</i> , 2018, 8, 11910-11925.	11.2	11
58	Obtaining Intrinsically Occupied Free-Space Superatom States in an Encapsulated Ca ₂ N Nanotube. <i>ACS Omega</i> , 2018, 3, 11966-11971.	3.5	3
59	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
60	Growth of boron nitride nanotubes from magnesium diboride catalysts. <i>Nanoscale</i> , 2018, 10, 13895-13901.	5.6	28
61	Rational Design of Two-dimensional Anode Materials: B ₂ S as a Strained Graphene. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4852-4856.	4.6	38
62	Atomically thin semiconducting penta-PdP ₂ and PdAs ₂ with ultrahigh carrier mobility. <i>Journal of Materials Chemistry C</i> , 2018, 6, 9055-9059.	5.5	39
63	Paleomagnetic constraints on the paleolatitude of the Lhasa block during the Early Cretaceous: Implications for the onset of India-Asia collision and latitudinal shortening estimates across Tibet and stable Asia. <i>Gondwana Research</i> , 2017, 41, 352-372.	6.0	49
64	First-Principles Study of Molecular Clusters Formed by Nitric Acid and Ammonia. <i>Journal of Physical Chemistry A</i> , 2017, 121, 661-668.	2.5	13
65	A Kinetic Pathway toward High-Density Ordered N Doping of Epitaxial Graphene on Cu(111) Using C ₅ NCl ₅ Precursors. <i>Journal of the American Chemical Society</i> , 2017, 139, 7196-7202.	13.7	16
66	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
67	Thickness-Dependent Adsorption of Melamine on Cu/Au(111) Films. <i>Journal of Physical Chemistry C</i> , 2017, 121, 7977-7984.	3.1	15
68	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
69	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
70	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
71	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
72	LT-STM Investigation of the Self-Assembled F ₁₆ CuPc-Corannulene Binary System on Ag (111) and Grap. <i>Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica</i> , 2017, 33, 627-632.	4.9	3

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73	The Nanoparticle Size Effect in Graphene Cutting: A Mechanism. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9918-9921.	13.8	28
74	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
75	Mo ₂ 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
76	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
77	Electride: from computational characterization to theoretical design. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2016, 6, 430-440.	14.6	41
78	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
79	Distinct molecule adsorption behaviors on warped nanographene C ₈₀ H ₃₀ : A theoretical study. <i>Carbon</i> , 2016, 100, 428-434.	10.3	20
80	Electronic and transport properties of graphene with grain boundaries. <i>RSC Advances</i> , 2016, 6, 1090-1097.	3.6	14
81	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
82	A Density Functional Study of the Nonlinear Optical Properties of Edge-Functionalized Nonplanar Nanographenes. <i>ChemPhysChem</i> , 2015, 16, 2783-2788.	2.1	21
83	Streamline based design guideline for deterministic microfluidic hydrodynamic single cell traps. <i>Biomicrofluidics</i> , 2015, 9, 024103.	2.4	19
84	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
85	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
86	Single-Molecule Imaging of Activated Nitrogen Adsorption on Individual Manganese Phthalocyanine. <i>Nano Letters</i> , 2015, 15, 3181-3188.	9.1	22
87	Aerobic Oxidation of Cyclohexane on Catalysts Based on Twinned and Single-Crystal Au ₇₅ Pd ₂₅ Bimetallic Nanocrystals. <i>Nano Letters</i> , 2015, 15, 2875-2880.	9.1	92
88	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
89	Reversible Tuning of Interfacial and Intramolecular Charge Transfer in Individual MnPc Molecules. <i>Nano Letters</i> , 2015, 15, 8091-8098.	9.1	12
90	Gas-phase dynamics in graphene growth by chemical vapour deposition. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22832-22836.	2.8	48

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91	<scp>HONPAS</scp>: A linear scaling open-source solution for large system simulations. International Journal of Quantum Chemistry, 2015, 115, 647-655.	2.0	34
92	Simultaneous detection of multiple biological targets using optimized microfluidic microsphere-trap arrays. Journal of Micro/ Nanolithography, MEMS, and MOEMS, 2014, 13, 1.	0.9	10
93	Mechanisms of Graphene Growth on Metal Surfaces: Theoretical Perspectives. Small, 2014, 10, 2136-2150.	10.0	73
94	Silicene as a highly sensitive molecule sensor for NH ₃ , NO and NO ₂ . Physical Chemistry Chemical Physics, 2014, 16, 6957.	2.8	221
95	Single molecule tunneling spectroscopy investigation of reversibly switched dipolar vanadyl phthalocyanine on graphite. Applied Physics Letters, 2014, 104, .	3.3	13
96	Density Functional Study of Nonlinear Optical Properties of Grossly Warped Nanographene C ₈₀ H ₃₀ . Journal of Physical Chemistry C, 2014, 118, 3313-3318.	3.1	27
97	Proposed Photosynthesis Method for Producing Hydrogen from Dissociated Water Molecules Using Incident Near-Infrared Light. Physical Review Letters, 2014, 112, 018301.	7.8	237
98	Remarkable chemical adsorption of manganese-doped titanate for direct carbon dioxide electrolysis. Journal of Materials Chemistry A, 2014, 2, 6904-6915.	10.3	137
99	A smartphone controlled handheld microfluidic liquid handling system. Lab on A Chip, 2014, 14, 4085-4092.	6.0	54
100	A first-principles study of gas adsorption on germanene. Physical Chemistry Chemical Physics, 2014, 16, 22495-22498.	2.8	232
101	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.	13.7	280
102	Bilayer Graphene Growth via a Penetration Mechanism. Journal of Physical Chemistry C, 2014, 118, 6201-6206.	3.1	44
103	Methanol-Selective Oxidation Pathways on Au Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 17511-17520.	3.1	21
104	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.	3.6	55
105	Elementary Process for CVD Graphene on Cu(110): Size-selective Carbon Clusters. Scientific Reports, 2014, 4, 4431.	3.3	30
106	Scanning tunneling microscopy and density functional theory combined studies of rutile TiO ₂ (1 1 0) surface chemistry: Watch surface processes at the atomic scale. International Journal of Quantum Chemistry, 2013, 113, 89-95.	2.0	7
107	Finite element simulations of hydrodynamic trapping in microfluidic particle-trap array systems. Biomicrofluidics, 2013, 7, 54108.	2.4	32
108	Helium separation via porous silicene based ultimate membrane. Nanoscale, 2013, 5, 9062.	5.6	96

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109	A computational infrared spectroscopic study of graphene oxide. <i>Journal of Chemical Physics</i> , 2013, 139, 084704.	3.0	14
110	Structural, electronic, and optical properties of hybrid silicene and graphene nanocomposite. <i>Journal of Chemical Physics</i> , 2013, 139, 154704.	3.0	84
111	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
112	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
113	Rectangular cmos differential MAGFET biosensor for magnetic particle detection. <i>IEEE Transactions on Magnetics</i> , 2013, 49, 4052-4055.	2.1	3
114	Porous silicene as a hydrogen purification membrane. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5753.	2.8	127
115	Paleomagnetic constraints on the Cenozoic kinematic evolution of the Pamir plateau from the Western Kunlun Shan foreland. <i>Tectonophysics</i> , 2013, 603, 257-271.	2.2	12
116	Nondecaying long range effect of surface decoration on the charge state of NV center in diamond. <i>Journal of Chemical Physics</i> , 2013, 138, 034702.	3.0	6
117	Flexible packaging of solid-state integrated circuit chips with elastomeric microfluidics. <i>Scientific Reports</i> , 2013, 3, .	3.3	83
118	Electronic and optical properties of graphene and graphitic ZnO nanocomposite structures. <i>Journal of Chemical Physics</i> , 2013, 138, 124706.	3.0	97
119	Diamond as an inert substrate of graphene. <i>Journal of Chemical Physics</i> , 2013, 138, 054701.	3.0	46
120	A first-principles study of ZnO polar surface growth: Adsorption of Zn _x O _y clusters. <i>Journal of Chemical Physics</i> , 2013, 139, 124704.	3.0	7
121	Orientation-sensitive nonlinear growth of graphene: An epitaxial growth mechanism determined by geometry. <i>Physical Review B</i> , 2013, 88, .	3.2	9
122	Diffusion and desorption of oxygen atoms on graphene. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 405301.	1.8	24
123	Optimization of microfluidic microsphere-trap arrays. <i>Biomicrofluidics</i> , 2013, 7, 14112.	2.4	28
124	High-Pressure Phase Favored by a Symmetry-Recognized Nanoconfinement Effect. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2154-2158.	4.6	2
125	Oxygen molecule dissociation on carbon nanostructures with different types of nitrogen doping. <i>Nanoscale</i> , 2012, 4, 1184-1189.	5.6	220
126	A first-principles prediction of two-dimensional superconductivity in pristine B2C single layers. <i>Nanoscale</i> , 2012, 4, 3032.	5.6	67

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127	Bipolar magnetic semiconductors: a new class of spintronics materials. <i>Nanoscale</i> , 2012, 4, 5680.	5.6	241
128	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
129	Lattice Mismatch Induced Nonlinear Growth of Graphene. <i>Journal of the American Chemical Society</i> , 2012, 134, 6045-6051.	13.7	88
130	Diamondization of chemically functionalized graphene and grapheneâ€“BN bilayers. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 8179.	2.8	52
131	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
132	Are Azafullerene Encapsulated Single-Walled Carbon Nanotubes n-Type Semiconductors?. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12760-12762.	3.1	12
133	STM studies of single molecules: molecular orbital aspects. <i>Chemical Communications</i> , 2011, 47, 2747.	4.1	10
134	Structure of Graphene Oxide: Thermodynamics versus Kinetics. <i>Journal of Physical Chemistry C</i> , 2011, 115, 11991-11995.	3.1	91
135	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
136	First-Principles Thermodynamics of Graphene Growth on Cu Surfaces. <i>Journal of Physical Chemistry C</i> , 2011, 115, 17782-17787.	3.1	317
137	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
138	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
139	Site-specific photocatalytic splitting of methanol on TiO ₂ (110). <i>Chemical Science</i> , 2010, 1, 575.	7.4	150
140	Discriminating early stage A ² 42 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
141	Linear scaling electronic structure calculations with numerical atomic basis set. <i>International Reviews in Physical Chemistry</i> , 2010, 29, 665-691.	2.3	23
142	Implementation of Exact Exchange with Numerical Atomic Orbitals. <i>Journal of Physical Chemistry A</i> , 2010, 114, 1039-1043.	2.5	19
143	First principles nuclear magnetic resonance signatures of graphene oxide. <i>Journal of Chemical Physics</i> , 2010, 133, 034502.	3.0	51
144	Single-Molecule Chemistry of Metal Phthalocyanine on Noble Metal Surfaces. <i>Accounts of Chemical Research</i> , 2010, 43, 954-962.	15.6	105

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145	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
146	Boron K4 crystal: a stable chiral three-dimensional sp ² network. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12420.	2.8	25
147	Single-stranded DNA adsorption on chiral molecule coated Au surface: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4431.	2.8	11
148	Density functional study on mechanism of CO oxidation with activated water on O/Au (111) surface. <i>Science Bulletin</i> , 2009, 54, 1973-1977.	9.0	7
149	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
150	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
151	A multi-color fast-switching microfluidic droplet dye laser. <i>Lab on A Chip</i> , 2009, 9, 2767.	6.0	177
152	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
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