Zhenyu Li

List of Publications by Year in Descending Order

179 papers	8,680 citations	48 h-index	89 g-index
189 ext. papers	9,776 ext. citations	6.7 avg, IF	6.37 L-index

#	Paper	IF	Citations
179	Understanding High-Temperature Chemical Reactions on Metal Surfaces: A Case Study on Equilibrium Concentration and Diffusivity of C H on a Cu(111) Surface.. *Jacs Au*, **2022**, 2, 443-452		2
178	Unveiling the Atomic Structure and Growth Dynamics of One-Dimensional Water on ZnO(10-10).. *Journal of Physical Chemistry Letters*, **2022**, 1554-1562	6.4	1
177	Computational characterization of nanosystems. *Chinese Journal of Chemical Physics*, **2022**, 35, 1-15	0.9	
176	The Important Role of Optical Absorption in Determining the Efficiency of Intermediate Band Solar Cells and a Design Principle for Perovskite Doping.. *Journal of Physical Chemistry Letters*, **2022**, 13, 2012-2018	6.4	1
175	Schottky and Ohmic Contacts at Tellurene/2D Metal Interfaces. *ACS Applied Electronic Materials*, **2022**, 4, 1082-1088	4	2
174	Reaction Mechanism and Strategy for Optimizing the Hydrogen Evolution Reaction on Single-Layer 1T' WSe and WTe Based on Grand Canonical Potential Kinetics. *ACS Applied Materials & Interfaces*, **2021**, 13, 55611-55620	9.5	2
173	Single Molecular Reaction of Water on a ZnO Surface. *Nano Letters*, **2021**, 21, 9567-9572	11.5	2
172	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	3.8	5
171	Hetero-site nucleation for growing twisted bilayer graphene with a wide range of twist angles. *Nature Communications*, **2021**, 12, 2391	17.4	31
170	Efficient Direct Band Gap Photovoltaic Material Predicted Via Doping Double Perovskites Cs2AgBiX6 (X = Cl, Br). *Journal of Physical Chemistry C*, **2021**, 125, 10868-10875	3.8	10
169	An efficient adaptive variational quantum solver of the Schrödinger equation based on reduced density matrices. *Journal of Chemical Physics*, **2021**, 154, 244112	3.9	3
168	Doping-controllable high temperature magnetic semiconductor. *Physica E: Low-Dimensional Systems and Nanostructures*, **2021**, 131, 114731	3	1
167	Atom by Atom Condensation of Sn Single Clusters within Gold-Phosphorus Metal-Inorganic Porous Networks. *Journal of Physical Chemistry Letters*, **2021**, 12, 745-751	6.4	3
166	The mobility and solvation structure of a hydroxyl radical in a water nanodroplet: a Born-Oppenheimer molecular dynamics study. *Physical Chemistry Chemical Physics*, **2021**, 23, 14628-14635	3.6	4
165	Promoted H2 splitting on ZnO by pre-adsorbed formic acid. *Journal of Catalysis*, **2021**, 400, 212-217	7.3	2
164	Intrinsic Descriptors for Coordination Environment and Synergistic Effects of Metal and Environment in Single-Atom-Catalyzed Carbon Dioxide Electroreduction. *Journal of Physical Chemistry C*, **2021**, 125, 18180-18186	3.8	2
163	Reaction between a NO Dimer and Dissolved SO: A New Mechanism for ONSO Formation and its Fate in Aerosol. *Journal of Physical Chemistry A*, **2021**, 125, 8468-8475	2.8	0

162	Equation-of-Motion Theory to Calculate Accurate Band Structures with a Quantum Computer. *Journal of Physical Chemistry Letters*, **2021**, 12, 8833-8840	6.4	2
161	Toward Epitaxial Growth of Misorientation-Free Graphene on Cu(111) Foils.. *ACS Nano*, **2021**,	16.7	4
160	Intrinsic ferromagnetic semiconductivity realized in a new MoS monolayer. *Physical Chemistry Chemical Physics*, **2020**, 22, 13363-13367	3.6	1
159	Designing Kagome Lattice from Potassium Atoms on Phosphorus-Gold Surface Alloy. *Nano Letters*, **2020**, 20, 5583-5589	11.5	9
158	Theoretical Insights into the Thermodynamics and Kinetics of Graphene Growth on Copper Surfaces. *Journal of Physical Chemistry C*, **2020**, 124, 16233-16247	3.8	9
157	Single Faceted Two-Dimensional Mo2C Electrocatalyst for Highly Efficient Nitrogen Fixation. *ACS Catalysis*, **2020**, 10, 7864-7870	13.1	33
156	Synthesis of Monolayer Blue Phosphorus Enabled by Silicon Intercalation. *ACS Nano*, **2020**, 14, 3687-3695	16.7	28
155	Steric Hindrance Effect in High-Temperature Reactions. *CCS Chemistry*, **2020**, 2, 460-467	7.2	13
154	Structure of Blue Phosphorus Grown on Au(111) Surface Revisited. *Journal of Physical Chemistry C*, **2020**, 124, 2024-2029	3.8	19
153	Coordinate activation in heterogeneous carbon dioxide reduction on Co-based molecular catalysts. *Applied Catalysis B: Environmental*, **2020**, 268, 118452	21.8	23
152	Dissociative adsorption and linear organization of formic acid on ZnO(1□0□1□0) surface. *Journal of Catalysis*, **2020**, 390, 109-116	7.3	5
151	Simulating Periodic Systems on a Quantum Computer Using Molecular Orbitals. *Journal of Chemical Theory and Computation*, **2020**, 16, 6904-6914	6.4	3
150	Spin□phonon coupling in NiO nanoparticle. *Journal of Applied Physics*, **2020**, 128, 133905	2.5	7
149	Half-filled intermediate bands in doped inorganic perovskites for solar cells. *Physical Chemistry Chemical Physics*, **2020**, 22, 23804-23809	3.6	5
148	Intrinsic ultra-wide completely spin-polarized state realized in a new CrO monolayer. *Physical Chemistry Chemical Physics*, **2020**, 22, 17038-17041	3.6	6
147	Molecular Mechanisms and Atmospheric Implications of Criegee Intermediate-Alcohol Chemistry in the Gas Phase and Aqueous Surface Environments. *Journal of Physical Chemistry A*, **2020**, 124, 8585-8593	2.8	4
146	On-Surface Synthesis of Nitrogen-Substituted Gold-Phosphorus Porous Network. *Chemistry of Materials*, **2020**, 32, 8561-8566	9.6	3
145	One-Dimensional Magnetic Order Stabilized in Edge-Reconstructed MoS Nanoribbon via Bias Voltage. *Journal of Physical Chemistry Letters*, **2020**, 11, 7531-7535	6.4	6

144	Descriptor-Based Design Principle for Two-Dimensional Single-Atom Catalysts: Carbon Dioxide Electroreduction. *Journal of Physical Chemistry Letters*, **2020**, 11, 3481-3487	6.4	34
143	Molecular mechanism of heterogeneous supramolecular catalysis of metal-free cucurbituril solid for epoxide alcoholysis. *Molecular Catalysis*, **2019**, 467, 1-8	3.3	5
142	Ion Conductivity Enhancement in Anti-Spinel Li3OBr with Intrinsic Vacancies. *Advanced Theory and Simulations*, **2019**, 2, 1800138	3.5	9
141	Transition-Metal Diboride: A New Family of Two-Dimensional Materials Designed for Selective CO2 Electroreduction. *Journal of Physical Chemistry C*, **2019**, 123, 16294-16299	3.8	25
140	Low-Temperature Heterolytic Adsorption of H2 on ZnO(101 0) Surface. *Journal of Physical Chemistry C*, **2019**, 123, 13283-13287	3.8	8
139	Rh Doping in Pd Nanocubes Optimizes the Adsorption of 3-Nitrostyrene towards Selective Hydrogenation of Vinyl Group. *ChemCatChem*, **2019**, 11, 2793-2798	5.2	4
138	Coordination polymer derived Ni based composite material with N-doped mesoporous carbon as matrix for pollutants removal. *Journal of Porous Materials*, **2019**, 26, 205-215	2.4	
137	Reversible Oxidation of Blue Phosphorus Monolayer on Au(111). *Nano Letters*, **2019**, 19, 5340-5346	11.5	21
136	Theoretical Insights into Li-Ion Transport in LiTa2PO8. *Journal of Physical Chemistry C*, **2019**, 123, 19282-19287	3.8	8
135	Boosting ionic conductivity in antiperovskite Li3OCl via defect engineering: Interstitial versus vacancy. *Physical Review Materials*, **2019**, 3,	3.2	7
134	Predictive design of intrinsic half-metallicity in zigzag tungsten dichalcogenide nanoribbons. *Physical Review B*, **2019**, 100,	3.3	3
133	Atomistic Simulations of Graphene Growth: From Kinetics to Mechanism. *Accounts of Chemical Research*, **2018**, 51, 728-735	24.3	20
132	Adsorption and Diffusion of CO on Clean and CO2-Precovered ZnO(101 0). *Journal of Physical Chemistry C*, **2018**, 122, 8919-8924	3.8	13
131	Sandwich-Like Nanosheets of a N-Doped Porous Carbon/Graphene Composite with Enhanced Electrochemical Properties for Lithium and Sodium Storage. *ChemElectroChem*, **2018**, 5, 694-700	4.3	9
130	Interfacial properties of black phosphorus/transition metal carbide van der Waals heterostructures. *Frontiers of Physics*, **2018**, 13, 1	3.7	15
129	Growth of boron nitride nanotubes from magnesium diboride catalysts. *Nanoscale*, **2018**, 10, 13895-13901	7.7	18
128	Rational Design of Two-dimensional Anode Materials: BS as a Strained Graphene. *Journal of Physical Chemistry Letters*, **2018**, 9, 4852-4856	6.4	25
127	Atomically thin semiconducting penta-PdP2 and PdAs2 with ultrahigh carrier mobility. *Journal of Materials Chemistry C*, **2018**, 6, 9055-9059	7.1	25

126	Doping-induced structural phase transition in cobalt diselenide enables enhanced hydrogen evolution catalysis. *Nature Communications*, **2018**, 9, 2533	17.4	244
125	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	13.1	6
124	Obtaining Intrinsically Occupied Free-Space Superatom States in an Encapsulated CaN Nanotube. *ACS Omega*, **2018**, 3, 11966-11971	3.9	3
123	Electron-phonon interaction in a Ca2N monolayer: Intrinsic mobility of electrene. *Physical Review B*, **2018**, 98,	3.3	11
122	In Situ Thermal Atomization To Convert Supported Nickel Nanoparticles into Surface-Bound Nickel Single-Atom Catalysts. *Angewandte Chemie - International Edition*, **2018**, 57, 14095-14100	16.4	206
121	In Situ Thermal Atomization To Convert Supported Nickel Nanoparticles into Surface-Bound Nickel Single-Atom Catalysts. *Angewandte Chemie*, **2018**, 130, 14291-14296	3.6	30
120	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	11.5	84
119	First-Principles Study of Molecular Clusters Formed by Nitric Acid and Ammonia. *Journal of Physical Chemistry A*, **2017**, 121, 661-668	2.8	9
118	A Kinetic Pathway toward High-Density Ordered N Doping of Epitaxial Graphene on Cu(111) Using CNCl Precursors. *Journal of the American Chemical Society*, **2017**, 139, 7196-7202	16.4	12
117	Growth of Quasi-Free-Standing Single-Layer Blue Phosphorus on Tellurium Monolayer Functionalized Au(111). *ACS Nano*, **2017**, 11, 4943-4949	16.7	92
116	Phosphorus Nanostripe Arrays on Cu(110): A Case Study to Understand the Substrate Effect on the Phosphorus thin Film Growth. *Advanced Materials Interfaces*, **2017**, 4, 1601167	4.6	13
115	Water on silicene: A hydrogen bond-autocatalyzed physisorption□chemisorption□dissociation transition. *Nano Research*, **2017**, 10, 2223-2233	10	14
114	Thickness-Dependent Adsorption of Melamine on Cu/Au(111) Films. *Journal of Physical Chemistry C*, **2017**, 121, 7977-7984	3.8	11
113	Contrasting Structural Reconstructions, Electronic Properties, and Magnetic Orderings along Different Edges of Zigzag Transition Metal Dichalcogenide Nanoribbons. *Nano Letters*, **2017**, 17, 1097-1101	11.5	60
112	Two-Dimensional Stoichiometric Boron Oxides as a Versatile Platform for Electronic Structure Engineering. *Journal of Physical Chemistry Letters*, **2017**, 8, 4347-4353	6.4	31
111	Dominant Kinetic Pathways of Graphene Growth in Chemical Vapor Deposition: The Role of Hydrogen. *Journal of Physical Chemistry C*, **2017**, 121, 25949-25955	3.8	47
110	Precursor Triggering Synthesis of Self-Coupled Sulfide Polymorphs with Enhanced Photoelectrochemical Properties. *Journal of the American Chemical Society*, **2016**, 138, 12913-12919	16.4	69
109	Electride: from computational characterization to theoretical design. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 430-440	7.9	31

108	Epitaxial Growth of Single Layer Blue Phosphorus: A New Phase of Two-Dimensional Phosphorus. *Nano Letters*, **2016**, 16, 4903-8	11.5	490
107	Distinct molecule adsorption behaviors on warped nanographene C80H30: A theoretical study. *Carbon*, **2016**, 100, 428-434	10.4	16
106	Electronic and transport properties of graphene with grain boundaries. *RSC Advances*, **2016**, 6, 1090-1097	3.7	13
105	Rücktitelbild: The Nanoparticle Size Effect in Graphene Cutting: A "Pac-Man" Mechanism (Angew. Chem. 34/2016). *Angewandte Chemie*, **2016**, 128, 10304-10304	3.6	
104	The Nanoparticle Size Effect in Graphene Cutting: A "Pac-Man" Mechanism. *Angewandte Chemie - International Edition*, **2016**, 55, 9918-21	16.4	22
103	The Nanoparticle Size Effect in Graphene Cutting: A "Pac-Man" Mechanism. *Angewandte Chemie*, **2016**, 128, 10072-10075	3.6	7
102	Mo2C nanoparticles embedded within bacterial cellulose-derived 3D N-doped carbon nanofiber networks for efficient hydrogen evolution. *NPG Asia Materials*, **2016**, 8, e288-e288	10.3	127
101	Single-molecule imaging of activated nitrogen adsorption on individual manganese phthalocyanine. *Nano Letters*, **2015**, 15, 3181-8	11.5	18
100	Aerobic Oxidation of Cyclohexane on Catalysts Based on Twinned and Single-Crystal Au75Pd25 Bimetallic Nanocrystals. *Nano Letters*, **2015**, 15, 2875-80	11.5	81
99	Ratio-controlled synthesis of CuNi octahedra and nanocubes with enhanced catalytic activity. *Journal of the American Chemical Society*, **2015**, 137, 14027-30	16.4	57
98	Reversible Tuning of Interfacial and Intramolecular Charge Transfer in Individual MnPc Molecules. *Nano Letters*, **2015**, 15, 8091-8	11.5	11
97	Gas-phase dynamics in graphene growth by chemical vapour deposition. *Physical Chemistry Chemical Physics*, **2015**, 17, 22832-6	3.6	34
96	Proposal of a general scheme to obtain room-temperature spin polarization in asymmetric antiferromagnetic semiconductors. *Physical Review B*, **2015**, 92,	3.3	15
95	A Density Functional Study of the Nonlinear Optical Properties of Edge-Functionalized Nonplanar Nanographenes. *ChemPhysChem*, **2015**, 16, 2783-2788	3.2	21
94	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	7.4	61
93	Elementary process for CVD graphene on Cu(110): size-selective carbon clusters. *Scientific Reports*, **2014**, 4, 4431	4.9	26
92	Mechanisms of graphene growth on metal surfaces: theoretical perspectives. *Small*, **2014**, 10, 2136-50	11	62
91	Silicene as a highly sensitive molecule sensor for NH3, NO and NO2. *Physical Chemistry Chemical Physics*, **2014**, 16, 6957-62	3.6	173

90	Single molecule tunneling spectroscopy investigation of reversibly switched dipolar vanadyl phthalocyanine on graphite. *Applied Physics Letters*, **2014**, 104, 113506	3.4	11
89	Density Functional Study of Nonlinear Optical Properties of Grossly Warped Nanographene C80H30. *Journal of Physical Chemistry C*, **2014**, 118, 3313-3318	3.8	21
88	Proposed photosynthesis method for producing hydrogen from dissociated water molecules using incident near-infrared light. *Physical Review Letters*, **2014**, 112, 018301	7.4	163
87	Graphene Growth: Mechanisms of Graphene Growth on Metal Surfaces: Theoretical Perspectives (Small 11/2014). *Small*, **2014**, 10, 2114-2114	11	1
86	Remarkable chemical adsorption of manganese-doped titanate for direct carbon dioxide electrolysis. *Journal of Materials Chemistry A*, **2014**, 2, 6904-6915	13	101
85	A first-principles study of gas adsorption on germanene. *Physical Chemistry Chemical Physics*, **2014**, 16, 22495-8	3.6	172
84	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, 13313-8	16.4	204
83	Bilayer Graphene Growth via a Penetration Mechanism. *Journal of Physical Chemistry C*, **2014**, 118, 6201-6206	4.8	39
82	Methanol-Selective Oxidation Pathways on Au Surfaces: A First-Principles Study. *Journal of Physical Chemistry C*, **2014**, 118, 17511-17520	3.8	19
81	Scanning tunneling microscopy and density functional theory combined studies of rutile TiO2(1 1 0) surface chemistry: Watch surface processes at the atomic scale. *International Journal of Quantum Chemistry*, **2013**, 113, 89-95	2.1	6
80	Cutting Graphitic Materials: A Promising Way to Prepare Graphene Nanoribbons **2013**, 79-99		
79	Helium separation via porous silicene based ultimate membrane. *Nanoscale*, **2013**, 5, 9062-6	7.7	82
78	A computational infrared spectroscopic study of graphene oxide. *Journal of Chemical Physics*, **2013**, 139, 084704	3.9	6
77	Structural, electronic, and optical properties of hybrid silicene and graphene nanocomposite. *Journal of Chemical Physics*, **2013**, 139, 154704	3.9	79
76	Hydrogenated bilayer wurtzite SiC nanofilms: a two-dimensional bipolar magnetic semiconductor material. *Physical Chemistry Chemical Physics*, **2013**, 15, 497-503	3.6	52
75	Surface and size effects on the charge state of NV center in nanodiamonds. *Computational and Theoretical Chemistry*, **2013**, 1021, 49-53	2	16
74	Porous silicene as a hydrogen purification membrane. *Physical Chemistry Chemical Physics*, **2013**, 15, 5753-7	3.6	110
73	Nondecaying long range effect of surface decoration on the charge state of NV center in diamond. *Journal of Chemical Physics*, **2013**, 138, 034702	3.9	6

72	Electronic and optical properties of graphene and graphitic ZnO nanocomposite structures. *Journal of Chemical Physics*, **2013**, 138, 124706	3.9	82
71	Diamond as an inert substrate of graphene. *Journal of Chemical Physics*, **2013**, 138, 054701	3.9	38
70	A first-principles study of ZnO polar surface growth: adsorption of Zn(x)O(y) clusters. *Journal of Chemical Physics*, **2013**, 139, 124704	3.9	6
69	Orientation-sensitive nonlinear growth of graphene: An epitaxial growth mechanism determined by geometry. *Physical Review B*, **2013**, 88,	3.3	8
68	Diffusion and desorption of oxygen atoms on graphene. *Journal of Physics Condensed Matter*, **2013**, 25, 405301	1.8	16
67	High-Pressure Phase Favored by a Symmetry-Recognized Nanoconfinement Effect. *Journal of Physical Chemistry Letters*, **2012**, 3, 2154-8	6.4	2
66	Oxygen molecule dissociation on carbon nanostructures with different types of nitrogen doping. *Nanoscale*, **2012**, 4, 1184-9	7.7	195
65	A first-principles prediction of two-dimensional superconductivity in pristine B□ single layers. *Nanoscale*, **2012**, 4, 3032-5	7.7	55
64	Bipolar magnetic semiconductors: a new class of spintronics materials. *Nanoscale*, **2012**, 4, 5680-5	7.7	162
63	Graphene Thickness Control via Gas-Phase Dynamics in Chemical Vapor Deposition. *Journal of Physical Chemistry C*, **2012**, 116, 10557-10562	3.8	59
62	Lattice mismatch induced nonlinear growth of graphene. *Journal of the American Chemical Society*, **2012**, 134, 6045-51	16.4	80
61	Diamondization of chemically functionalized graphene and graphene-BN bilayers. *Physical Chemistry Chemical Physics*, **2012**, 14, 8179-84	3.6	48
60	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. *Journal of Physical Chemistry C*, **2012**, 116, 3142-3146	3.8	88
59	Graphene Oxide: Theoretical Perspectives **2012**, 69-84		6
58	STM studies of single molecules: molecular orbital aspects. *Chemical Communications*, **2011**, 47, 2747-62	5.8	8
57	Structure of Graphene Oxide: Thermodynamics versus Kinetics. *Journal of Physical Chemistry C*, **2011**, 115, 11991-11995	3.8	83
56	Low-temperature growth of graphene by chemical vapor deposition using solid and liquid carbon sources. *ACS Nano*, **2011**, 5, 3385-90	16.7	304
55	First-Principles Thermodynamics of Graphene Growth on Cu Surfaces. *Journal of Physical Chemistry C*, **2011**, 115, 17782-17787	3.8	276

54	Density functional predictions of new silicon allotropes: Electronic properties and potential applications to Li-battery anode materials. *Solid State Communications*, **2011**, 151, 1228-1230	1.6	18
53	Are Azafullerene Encapsulated Single-Walled Carbon Nanotubes n-Type Semiconductors?. *Journal of Physical Chemistry C*, **2011**, 115, 12760-12762	3.8	11
52	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	3.9	20
51	Discriminating early stage A{beta}42 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, 15687-92	11.5	36
50	Linear scaling electronic structure calculations with numerical atomic basis set. *International Reviews in Physical Chemistry*, **2010**, 29, 665-691	7	15
49	Implementation of exact exchange with numerical atomic orbitals. *Journal of Physical Chemistry A*, **2010**, 114, 1039-43	2.8	16
48	First principles nuclear magnetic resonance signatures of graphene oxide. *Journal of Chemical Physics*, **2010**, 133, 034502	3.9	45
47	Single-molecule chemistry of metal phthalocyanine on noble metal surfaces. *Accounts of Chemical Research*, **2010**, 43, 954-62	24.3	98
46	Communication: Coalescence of carbon atoms on Cu (111) surface: Emergence of a stable bridging-metal structure motif. *Journal of Chemical Physics*, **2010**, 133, 071101	3.9	67
45	Boron K4 crystal: a stable chiral three-dimensional sp(2) network. *Physical Chemistry Chemical Physics*, **2010**, 12, 12420-2	3.6	24
44	Single-stranded DNA adsorption on chiral molecule coated Au surface: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2010**, 12, 4431-4	3.6	9
43	Site-specific photocatalytic splitting of methanol on TiO2(110). *Chemical Science*, **2010**, 1, 575	9.4	143
42	Density functional study on mechanism of CO oxidation with activated water on O/Au (111) surface. *Science Bulletin*, **2009**, 54, 1973-1977	10.6	6
41	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	3.8	11
40	First Principles Study on the Geometric and Electronic Structures of the FeO/Pt(111) Surface. *Journal of Physical Chemistry C*, **2009**, 113, 8302-8305	3.8	33
39	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	3.8	122
38	How graphene is cut upon oxidation?. *Journal of the American Chemical Society*, **2009**, 131, 6320-1	16.4	289
37	Oxidation states of graphene: insights from computational spectroscopy. *Journal of Chemical Physics*, **2009**, 131, 244505	3.9	84

36	A density functional study on cationic Au(n)Cu(m)+ clusters and their monocarbonyls. *Physical Chemistry Chemical Physics*, **2009**, 11, 2329-34	3.6	32
35	Rectifying effect in polar conjugated molecular junctions: a first-principles study. *Journal of Nanoscience and Nanotechnology*, **2009**, 9, 774-8	1.3	20
34	A first-principles study of NO adsorption and oxidation on Au(111) surface. *Journal of Chemical Physics*, **2008**, 129, 134708	3.9	46
33	Half-metallicity in edge-modified zigzag graphene nanoribbons. *Journal of the American Chemical Society*, **2008**, 130, 4224-5	16.4	587
32	Half-metallicity in hybrid BCN nanoribbons. *Journal of Chemical Physics*, **2008**, 129, 084712	3.9	129
31	Electronic structures of SiC nanoribbons. *Journal of Chemical Physics*, **2008**, 129, 174114	3.9	199
30	Electronic Structures of Defective Boron Nitride Nanotubes under Transverse Electric Fields. *Journal of Physical Chemistry C*, **2008**, 112, 8424-8428	3.8	28
29	MAGNETISM IN GRAPHENE SYSTEMS. *Nano*, **2008**, 03, 433-442	1.1	61
28	Probing electron correlations in molecules by two-dimensional coherent optical spectroscopy. *Journal of the American Chemical Society*, **2008**, 130, 3509-15	16.4	27
27	Detecting a Molecule–Surface Hybrid State by an Fe-Coated Tip with a Non-s-Like Orbital. *Journal of Physical Chemistry C*, **2008**, 112, 15603-15606	3.8	14
26	A first principles study on organic molecule encapsulated boron nitride nanotubes. *Journal of Chemical Physics*, **2008**, 128, 164701	3.9	22
25	Electronic structures of organic molecule encapsulated BN nanotubes under transverse electric field. *Journal of Chemical Physics*, **2008**, 129, 024710	3.9	14
24	Protonation effects on electron transport through diblock molecular junctions: A theoretical study. *Science in China Series B: Chemistry*, **2008**, 51, 1159-1165		6
23	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	2.5	15
22	Oxygen adsorption on Zr(0 0 0 1) surfaces: Density functional calculations and a multiple-layer adsorption model. *Surface Science*, **2008**, 602, 2212-2216	1.8	22
21	First-principles simulation of amide and aromatic side chain ultraviolet spectroscopy of a cyclic dipeptide. *Journal of Physical Chemistry A*, **2007**, 111, 11579-83	2.8	11
20	Will zigzag graphene nanoribbon turn to half metal under electric field?. *Applied Physics Letters*, **2007**, 91, 243116	3.4	285
19	Two Dimensional Electronic Correlation Spectroscopy of the npi* and pipi* Protein Backbone Transitions: A Simulation Study. *Chemical Physics*, **2007**, 341, 29-36	2.3	27

18	Nature of well-defined conductance of amine-anchored molecular junctions: Density functional calculations. *Physical Review B*, **2007**, 76,	3.3	71
17	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	1.8	8
16	Linear scaling calculation of maximally localized Wannier functions with atomic basis set. *Journal of Chemical Physics*, **2006**, 124, 234108	3.9	11
15	Self-similarity of single-channel transmission for electron transport in nanowires. *Journal of Chemical Physics*, **2006**, 124, 104703	3.9	3
14	CHARGE AND SPIN ORDERING IN Na0.5CoO2 FROM THE HYBRID DENSITY FUNCTIONAL STUDY. *Journal of Theoretical and Computational Chemistry*, **2006**, 05, 515-522	1.8	
13	Dithiocarbamate anchoring in molecular wire junctions: a first principles study. *Journal of Physical Chemistry B*, **2006**, 110, 9893-8	3.4	72
12	Orbital interaction mechanisms of conductance enhancement and rectification by dithiocarboxylate anchoring group. *Journal of Physical Chemistry B*, **2006**, 110, 19116-20	3.4	47
11	Geometrical, electronic, and magnetic properties of Na0.5CoO2 from first principles. *Physical Review B*, **2005**, 71,	3.3	18
10	A first-principles study on quasi-1D alkali metal chains within zeolite channels. *Journal of Chemical Physics*, **2004**, 120, 9725-8	3.9	7
9	Is mayenite without clathrated oxygen an inorganic electride?. *Angewandte Chemie - International Edition*, **2004**, 43, 6479-82	16.4	63
8	Is Mayenite without Clathrated Oxygen an Inorganic Electride?. *Angewandte Chemie*, **2004**, 116, 6641-6644	3.6	3
7	Inorganic electrides. *Chemistry - A European Journal*, **2004**, 10, 1592-6	4.8	16
6	Theoretical study of nitric oxide adsorption on Au clusters. *Journal of Chemical Physics*, **2004**, 121, 2558-62	3.9	74
5	Adsorption energies of molecular oxygen on Au clusters. *Journal of Chemical Physics*, **2004**, 120, 9594-600	3.9	149
4	Electron-phonon coupling in a boron-doped diamond superconductor. *Physical Review B*, **2004**, 70,	3.3	122
3	Inorganic electride: theoretical study on structural and electronic properties. *Journal of the American Chemical Society*, **2003**, 125, 6050-1	16.4	35
2	Effects of discrete energy levels on single-electron tunneling in coupled metal particles. *Applied Physics Letters*, **2003**, 82, 3767-3769	3.4	27
1	Disorder and suppression of quantum confinement effects in Pd nanoparticles. *Physical Review Letters*, **2003**, 90, 246803	7.4	19