Jin-Long Yang

List of Publications by Year
in descending order

526 papers	38,057 citations	2423 97 h-index	4419 172 g-index
533 all docs	533 docs citations	533 times ranked	31471 citing authors

#	Article	IF	Citations
1	Partially oxidized atomic cobalt layers for carbon dioxide electroreduction to liquid fuel. Nature, 2016, 529, 68-71.	13.7	1,565
2	Metallic Few-Layered VS₂ Ultrathin Nanosheets: High Two-Dimensional Conductivity for In-Plane Supercapacitors. Journal of the American Chemical Society, 2011, 133, 17832-17838.	6.6	1,014
3	Regulation of Coordination Number over Single Co Sites: Triggering the Efficient Electroreduction of CO₂. Angewandte Chemie - International Edition, 2018, 57, 1944-1948.	7.2	888
4	Two-Dimensional Boron Monolayer Sheets. ACS Nano, 2012, 6, 7443-7453.	7.3	690
5	Half-Metallicity in Edge-Modified Zigzag Graphene Nanoribbons. Journal of the American Chemical Society, 2008, 130, 4224-4225.	6.6	640
6	Identification of single-atom active sites in carbon-based cobalt catalysts during electrocatalytic hydrogen evolution. Nature Catalysis, 2019, 2, 134-141.	16.1	629
7	Controlling the Kondo Effect of an Adsorbed Magnetic Ion Through Its Chemical Bonding. Science, 2005, 309, 1542-1544.	6.0	594
8	Bottom-up precise synthesis of stable platinum dimers on graphene. Nature Communications, 2017, 8, 1070.	5.8	466
9	Atomically dispersed iron hydroxide anchored on Pt for preferential oxidation of CO in H2. Nature, 2019, 565, 631-635.	13.7	423
10	Dynamic oxygen adsorption on single-atomic Ruthenium catalyst with high performance for acidic oxygen evolution reaction. Nature Communications, 2019, 10, 4849.	5.8	416
11	Intrinsic Electric Fields in Two-dimensional Materials Boost the Solar-to-Hydrogen Efficiency for Photocatalytic Water Splitting. Nano Letters, 2018, 18, 6312-6317.	4.5	391
12	Giant Moisture Responsiveness of VS₂ Ultrathin Nanosheets for Novel Touchless Positioning Interface. Advanced Materials, 2012, 24, 1969-1974.	11.1	364
13	Low-Temperature Growth of Graphene by Chemical Vapor Deposition Using Solid and Liquid Carbon Sources. ACS Nano, 2011, 5, 3385-3390.	7.3	353
14	Half-Metallicity in MnPSe₃ Exfoliated Nanosheet with Carrier Doping. Journal of the American Chemical Society, 2014, 136, 11065-11069.	6.6	353
15	Enhanced photocatalytic mechanism for the hybrid g-C₃N₄/MoS₂ nanocomposite. Journal of Materials Chemistry A, 2014, 2, 7960-7966.	5.2	347
16	First-principles design of spintronics materials. National Science Review, 2016, 3, 365-381.	4.6	344
17	CrXTe₃(X = Si, Ge) nanosheets: two dimensional intrinsic ferromagnetic semiconductors. Journal of Materials Chemistry C, 2014, 2, 7071.	2.7	332
18	How Graphene Is Cut upon Oxidation?. Journal of the American Chemical Society, 2009, 131, 6320-6321.	6.6	323

#	Article	IF	Citations
19	First-Principles Thermodynamics of Graphene Growth on Cu Surfaces. Journal of Physical Chemistry C, 2011, 115, 17782-17787.	1.5	317
20	Understanding of Strain Effects in the Electrochemical Reduction of CO₂: Using Pd Nanostructures as an Ideal Platform. Angewandte Chemie - International Edition, 2017, 56, 3594-3598.	7.2	303
21	Conjugated Microporous Polymer Nanosheets for Overall Water Splitting Using Visible Light. Advanced Materials, 2017, 29, 1702428.	11.1	302
22	Will zigzag graphene nanoribbon turn to half metal under electric field?. Applied Physics Letters, 2007, 91, .	1.5	299
23	Visualizing coherent intermolecular dipoleâ€“dipole coupling in real space. Nature, 2016, 531, 623-627.	13.7	284
24	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
25	Hydrogen-Incorporated TiS₂ Ultrathin Nanosheets with Ultrahigh Conductivity for Stamp-Transferrable Electrodes. Journal of the American Chemical Society, 2013, 135, 5144-5151.	6.6	273
26	Atomicâ€Level Insight into Optimizing the Hydrogen Evolution Pathway over a Co₁â€N₄ Singleâ€Site Photocatalyst. Angewandte Chemie - International Edition, 2017, 56, 12191-12196.	7.2	269
27	Achieving Remarkable Activity and Durability toward Oxygen Reduction Reaction Based on Ultrathin Rh-Doped Pt Nanowires. Journal of the American Chemical Society, 2017, 139, 8152-8159.	6.6	265
28	Structural isomerism in gold nanoparticles revealed by X-ray crystallography. Nature Communications, 2015, 6, 8667.	5.8	258
29	Material Design for Photocatalytic Water Splitting from a Theoretical Perspective. Advanced Materials, 2018, 30, e1802106.	11.1	258
30	Single Mo₁(Cr₁) Atom on Nitrogen-Doped Graphene Enables Highly Selective Electroreduction of Nitrogen into Ammonia. ACS Catalysis, 2019, 9, 3419-3425.	5.5	258
31	Highly Efficient Photocatalytic Water Splitting over Edge-Modified Phosphorene Nanoribbons. Journal of the American Chemical Society, 2017, 139, 15429-15436.	6.6	244
32	Regulation of Coordination Number over Single Co Sites: Triggering the Efficient Electroreduction of CO₂. Angewandte Chemie, 2018, 130, 1962-1966.	1.6	244
33	Bipolar magnetic semiconductors: a new class of spintronics materials. Nanoscale, 2012, 4, 5680.	2.8	241
34	Wet Electrons at the H2O/TiO2(110) Surface. Science, 2005, 308, 1154-1158.	6.0	239
35	Distinguishing adjacent molecules on a surface using plasmon-enhanced Raman scattering. Nature Nanotechnology, 2015, 10, 865-869.	15.6	239
36	Proposed Photosynthesis Method for Producing Hydrogen from Dissociated Water Molecules Using Incident Near-Infrared Light. Physical Review Letters, 2014, 112, 018301.	2.9	237

#	Article	IF	Citations
37	A first-principles study of gas adsorption on germanene. Physical Chemistry Chemical Physics, 2014, 16, 22495-22498.	1.3	232
38	Electronic structures of SiC nanoribbons. Journal of Chemical Physics, 2008, 129, 174114.	1.2	222
39	Silicene as a highly sensitive molecule sensor for NH3, NO and NO2. Physical Chemistry Chemical Physics, 2014, 16, 6957.	1.3	221
40	Oxygen molecule dissociation on carbon nanostructures with different types of nitrogen doping. Nanoscale, 2012, 4, 1184-1189.	2.8	220
41	Graphene nanoribbon as a negative differential resistance device. Applied Physics Letters, 2009, 94, .	1.5	219
42	Unconventional pâ€"d Hybridization Interaction in PtGa Ultrathin Nanowires Boosts Oxygen Reduction Electrocatalysis. Journal of the American Chemical Society, 2019, 141, 18083-18090.	6.6	216
43	Defects in Phosphorene. Journal of Physical Chemistry C, 2015, 119, 20474-20480.	1.5	215
44	Mono-cadmium vs Mono-mercury Doping of Au₂₅ Nanoclusters. Journal of the American Chemical Society, 2015, 137, 15350-15353.	6.6	211
45	A Theoretical Study of Single-Atom Catalysis of CO Oxidation Using Au Embedded 2D h-BN Monolayer: A CO-Promoted O2 Activation. Scientific Reports, 2014, 4, 5441.	1.6	211
46	Stable Metallic 1Tâ€WS₂ Nanoribbons Intercalated with Ammonia Ions: The Correlation between Structure and Electrical/Optical Properties. Advanced Materials, 2015, 27, 4837-4844.	11.1	207
47	A Simple Molecular Design Strategy for Two-Dimensional Covalent Organic Framework Capable of Visible-Light-Driven Water Splitting. Journal of the American Chemical Society, 2020, 142, 4508-4516.	6.6	207
48	Ultrafast Interfacial Proton-Coupled Electron Transfer. Science, 2006, 311, 1436-1440.	6.0	206
49	Mono-Mercury Doping of Au₂₅ and the HOMO/LUMO Energies Evaluation Employing Differential Pulse Voltammetry. Journal of the American Chemical Society, 2015, 137, 9511-9514.	6.6	206
50	One-Dimensional Transition Metalâ^'Benzene Sandwich Polymers:Â Possible Ideal Conductors for Spin Transport. Journal of the American Chemical Society, 2006, 128, 2310-2314.	6.6	202
51	Room-Temperature Ferromagnetism in Two-Dimensional Fe₂Si Nanosheet with Enhanced Spin-Polarization Ratio. Nano Letters, 2017, 17, 2771-2777.	4.5	200
52	The electronic structure of oxygen atom vacancy and hydroxyl impurity defects on titanium dioxide (110) surface. Journal of Chemical Physics, 2009, 130, 124502.	1.2	197
53	Role of point defects on the reactivity of reconstructed anatase titanium dioxide (001) surface. Nature Communications, 2013, 4, 2214.	5.8	184
54	CO₂ Capture on <i>h</i>-BN Sheet with High Selectivity Controlled by External Electric Field. Journal of Physical Chemistry C, 2015, 119, 6912-6917.	1.5	183

#	Article	IF	Citations
55	Strain effect on electronic structures of graphene nanoribbons: A first-principles study. Journal of Chemical Physics, 2008, 129, 074704.	1.2	182
56	Tunable Magnetism in a Nonmetal-Substituted ZnO Monolayer: A First-Principles Study. Journal of Physical Chemistry C, 2012, 116, 11336-11342.	1.5	180
57	Effects of stacking order, layer number and external electric field on electronic structures of few-layer C₂N-h2D. Nanoscale, 2015, 7, 14062-14070.	2.8	177
58	Edge-Modified Phosphorene Nanoflake Heterojunctions as Highly Efficient Solar Cells. Nano Letters, 2016, 16, 1675-1682.	4.5	176
59	Adding Two Active Silver Atoms on Au₂₅ Nanoparticle. Nano Letters, 2015, 15, 1281-1287.	4.5	171
60	Observation of Photocatalytic Dissociation of Water on Terminal Ti Sites of TiO₂(110)-1 <i>Ã—</i> 1 Surface. Journal of the American Chemical Society, 2012, 134, 9978-9985.	6.6	160
61	One-Nanometer-Thick PtNiRh Trimetallic Nanowires with Enhanced Oxygen Reduction Electrocatalysis in Acid Media: Integrating Multiple Advantages into One Catalyst. Journal of the American Chemical Society, 2018, 140, 16159-16167.	6.6	160
62	Sub-nanometre control of the coherent interaction between a single molecule and a plasmonic nanocavity. Nature Communications, 2017, 8, 15225.	5.8	158
63	Molecular Oxygen Adsorption Behaviors on the Rutile TiO₂(110)-1Ã—1 Surface: An in Situ Study with Low-Temperature Scanning Tunneling Microscopy. Journal of the American Chemical Society, 2011, 133, 2002-2009.	6.6	155
64	A First-Principles Study on Electron Donor and Acceptor Molecules Adsorbed on Phosphorene. Journal of Physical Chemistry C, 2015, 119, 2871-2878.	1.5	152
65	Sub-nanometre resolution in single-molecule photoluminescence imaging. Nature Photonics, 2020, 14, 693-699.	15.6	152
66	Two-dimensional van der Waals heterojunctions for functional materials and devices. Journal of Materials Chemistry C, 2017, 5, 12289-12297.	2.7	151
67	Mechanism for Negative Differential Resistance in Molecular Electronic Devices: Local Orbital Symmetry Matching. Physical Review Letters, 2007, 99, 146803.	2.9	150
68	Site-specific photocatalytic splitting of methanol on TiO2(110). Chemical Science, 2010, 1, 575.	3.7	150
69	Î´-Phosphorene: a two dimensional material with a highly negative Poisson's ratio. Nanoscale, 2017, 9, 850-855.	2.8	150
70	Rational Design of Cathode Structure for High Rate Performance Lithiumâ€"Sulfur Batteries. Nano Letters, 2015, 15, 5443-5448.	4.5	147
71	Negative differential-resistance device involving two C60 molecules. Applied Physics Letters, 2000, 77, 3595-3597.	1.5	136
72	Half-metallicity in hybrid BCN nanoribbons. Journal of Chemical Physics, 2008, 129, 084712.	1.2	133

#	Article	IF	Citations
73	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
74	Mn₂C monolayer: a 2D antiferromagnetic metal with high NÃ©el temperature and large spinâ€“orbit coupling. Nanoscale, 2016, 8, 12939-12945.	2.8	131
75	New insight into the electronic shell of Au38(SR)24: a superatomic molecule. Nanoscale, 2013, 5, 1475.	2.8	128
76	Single layer of MX₃ (M = Ti, Zr; X = S, Se, Te): a new platform for nano-electronics and optics. Physical Chemistry Chemical Physics, 2015, 17, 18665-18669.	1.3	128
77	Porous silicene as a hydrogen purification membrane. Physical Chemistry Chemical Physics, 2013, 15, 5753.	1.3	127
78	Semihydrogenated BN Sheet: A Promising Visible-light Driven Photocatalyst for Water Splitting. Scientific Reports, 2013, 3, 1858.	1.6	127
79	Azide Passivation of Black Phosphorus Nanosheets: Covalent Functionalization Affords Ambient Stability Enhancement. Angewandte Chemie - International Edition, 2019, 58, 1479-1483.	7.2	123
80	Band-gap scaling of graphene nanohole superlattices. Physical Review B, 2009, 80, .	1.1	121
81	â€œNarrowâ€•Graphene Nanoribbons Made Easier by Partial Hydrogenation. Nano Letters, 2009, 9, 4025-4030.	4.5	120
82	Structures and magnetism of mono-palladium and mono-platinum doped Au₂₅(PET)₁₈nanoclusters. Chemical Communications, 2016, 52, 9873-9876.	2.2	120
83	Crystal and Solution Photoluminescence of MAg₂₄(SR)₁₈ (M = Ag/Pd/Pt/Au) Nanoclusters and Some Implications for the Photoluminescence Mechanisms. Journal of Physical Chemistry C, 2017, 121, 13848-13853.	1.5	120
84	Two-Dimensional Phosphorus Porous Polymorphs with Tunable Band Gaps. Journal of the American Chemical Society, 2016, 138, 7091-7098.	6.6	119
85	The gâ€C₃N₄/C₂N Nanocomposite: A gâ€C₃N₄â€Based Waterâ€Splitting Photocatalyst with Enhanced Energy Efficiency. ChemPhysChem, 2016, 17, 2100-2104.	1.0	118
86	Tunable Schottky contacts in hybrid grapheneâ€“phosphorene nanocomposites. Journal of Materials Chemistry C, 2015, 3, 4756-4761.	2.7	116
87	Electronic Structures and Magnetic Properties of GaN Sheets and Nanoribbons. Journal of Physical Chemistry C, 2010, 114, 11390-11394.	1.5	115
88	Theoretical study of small two-dimensional gold clusters. Physical Review B, 2003, 67, .	1.1	114
89	Effects of interlayer coupling and electric fields on the electronic structures of graphene and MoS₂heterobilayers. Journal of Materials Chemistry C, 2016, 4, 1776-1781.	2.7	114
90	Direct Z-Scheme Water Splitting Photocatalyst Based on Two-Dimensional Van Der Waals Heterostructures. Journal of Physical Chemistry Letters, 2018, 9, 5419-5424.	2.1	114

#	Article	IF	Citations
91	Superatom Networks in Thiolateâ€Protected Gold Nanoparticles. Angewandte Chemie - International Edition, 2013, 52, 9035-9039.	7.2	113
92	Highly Confined Water: Two-Dimensional Ice, Amorphous Ice, and Clathrate Hydrates. Accounts of Chemical Research, 2014, 47, 2505-2513.	7.6	113
93	Understanding of Strain Effects in the Electrochemical Reduction of CO₂: Using Pd Nanostructures as an Ideal Platform. Angewandte Chemie, 2017, 129, 3648-3652.	1.6	112
94	Two-dimensional van der Waals nanocomposites as Z-scheme type photocatalysts for hydrogen production from overall water splitting. Journal of Materials Chemistry A, 2016, 4, 18892-18898.	5.2	108
95	Direct hydrothermal synthesis of monoclinic VO2(M) single-domain nanorods on large scale displaying magnetocaloric effect. Journal of Materials Chemistry, 2011, 21, 4509.	6.7	106
96	Single-Molecule Chemistry of Metal Phthalocyanine on Noble Metal Surfaces. Accounts of Chemical Research, 2010, 43, 954-962.	7.6	105
97	Why the Band Gap of Graphene Is Tunable on Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2012, 116, 3142-3146.	1.5	103
98	Half-Metallicity in Organic Single Porous Sheets. Journal of the American Chemical Society, 2012, 134, 5718-5721.	6.6	101
99	2D Heterostructured Nanofluidic Channels for Enhanced Desalination Performance of Graphene Oxide Membranes. ACS Nano, 2021, 15, 7586-7595.	7.3	101
100	Hydrogen adsorption on zigzag (8,0) boron nitride nanotubes. Journal of Chemical Physics, 2004, 121, 8481.	1.2	97
101	Electronic and optical properties of graphene and graphitic ZnO nanocomposite structures. Journal of Chemical Physics, 2013, 138, 124706.	1.2	97
102	Activating Edge Sites on Pd Catalysts for Selective Hydrogenation of Acetylene via Selective Ga₂O₃ Decoration. ACS Catalysis, 2016, 6, 3700-3707.	5.5	97
103	Icosahedral B12-containing coreâ€“shell structures of B80. Chemical Communications, 2010, 46, 3878.	2.2	96
104	Half-Metallicity in Hybrid Graphene/Boron Nitride Nanoribbons with Dihydrogenated Edges. Journal of Physical Chemistry C, 2011, 115, 9442-9450.	1.5	96
105	Helium separation via porous silicene based ultimate membrane. Nanoscale, 2013, 5, 9062.	2.8	96
106	Band Structure Tuning of TiO₂ for Enhanced Photoelectrochemical Water Splitting. Journal of Physical Chemistry C, 2014, 118, 7451-7457.	1.5	95
107	Al_{<i>x</i>}C Monolayer Sheets: Two-Dimensional Networks with Planar Tetracoordinate Carbon and Potential Applications as Donor Materials in Solar Cell. Journal of Physical Chemistry Letters, 2014, 5, 2058-2065.	2.1	95
108	Intrinsic Quantum Anomalous Hall Effect with In-Plane Magnetization: Searching Rule and Material Prediction. Physical Review Letters, 2018, 121, 246401.	2.9	95

#	Article	IF	Citations
109	Ferroelectric hexagonal and rhombic monolayer ice phases. Chemical Science, 2014, 5, 1757-1764.	3.7	94
110	Chiral selective tunneling induced negative differential resistance in zigzag graphene nanoribbon: A theoretical study. Applied Physics Letters, 2008, 92, .	1.5	93
111	Electrically driven single-photon emission from an isolated single molecule. Nature Communications, 2017, 8, 580.	5.8	92
112	Theoretical study of the molecular and electronic structure of methanol on a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2009, 80, .	1.1	91
113	Structure of Graphene Oxide: Thermodynamics versus Kinetics. Journal of Physical Chemistry C, 2011, 115, 11991-11995.	1.5	91
114	Visually constructing the chemical structure of a single molecule by scanning Raman picoscopy. National Science Review, 2019, 6, 1169-1175.	4.6	91
115	Oxidation of a two-dimensional hexagonal boron nitride monolayer: a first-principles study. Physical Chemistry Chemical Physics, 2012, 14, 5545.	1.3	90
116	Bimetal Doping in Nanoclusters: Synergistic or Counteractive?. Chemistry of Materials, 2016, 28, 8240-8247.	3.2	90
117	Two-dimensional multilayer M₂CO₂(M = Sc, Zr, Hf) as photocatalysts for hydrogen production from water splitting: a first principles study. Journal of Materials Chemistry A, 2017, 5, 24972-24980.	5.2	90
118	Quasi Pd1Ni single-atom surface alloy catalyst enables hydrogenation of nitriles to secondary amines. Nature Communications, 2019, 10, 4998.	5.8	90
119	Highly-efficient heterojunction solar cells based on two-dimensional tellurene and transition metal dichalcogenides. Journal of Materials Chemistry A, 2019, 7, 7430-7436.	5.2	90
120	Atomic-Level Construction of Tensile-Strained PdFe Alloy Surface toward Highly Efficient Oxygen Reduction Electrocatalysis. Nano Letters, 2020, 20, 1403-1409.	4.5	89
121	High-performance photocatalytic nonoxidative conversion of methane to ethane and hydrogen by heteroatoms-engineered TiO2. Nature Communications, 2022, 13, 2806.	5.8	89
122	Design and control of electron transport properties of single molecules. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 15259-15263.	3.3	88
123	Oxidation states of graphene: Insights from computational spectroscopy. Journal of Chemical Physics, 2009, 131, 244505.	1.2	88
124	Shape-Dependent Reducibility of Cuprous Oxide Nanocrystals. Journal of Physical Chemistry C, 2010, 114, 6676-6680.	1.5	88
125	Lattice Mismatch Induced Nonlinear Growth of Graphene. Journal of the American Chemical Society, 2012, 134, 6045-6051.	6.6	88
126	Room-Temperature Half-Metallicity in La(Mn,Zn)AsO Alloy via Element Substitutions. Journal of the American Chemical Society, 2014, 136, 5664-5669.	6.6	88

#	Article	IF	Citations
127	First-principles study of two-dimensional van der Waals heterojunctions. Computational Materials Science, 2016, 112, 518-526.	1.4	88
128	What Are the Adsorption Sites for CO on the Reduced TiO₂(110)-1 Ã— 1 Surface?. Journal of the American Chemical Society, 2009, 131, 7958-7959.	6.6	87
129	Ultrahigh Infrared Photoresponse from Coreâ€"Shell Singleâ€Domainâ€VO₂/V₂O₅ Heterostructure in Nanobeam. Advanced Functional Materials, 2014, 24, 1821-1830.	7.8	87
130	Communication: New insight into electronic shells of metal clusters: Analogues of simple molecules. Journal of Chemical Physics, 2013, 138, 141101.	1.2	86
131	Understanding Single-Atom Catalysis in View of Theory. Jacs Au, 2021, 1, 2130-2145.	3.6	86
132	Hexagonal Cu2SnS3 with metallic character: Another category of conducting sulfides. Applied Physics Letters, 2007, 91, .	1.5	85
133	Structural, electronic, and optical properties of hybrid silicene and graphene nanocomposite. Journal of Chemical Physics, 2013, 139, 154704.	1.2	84
134	Blockage of ultrafast and directional diffusion of Li atoms on phosphorene with intrinsic defects. Nanoscale, 2016, 8, 4001-4006.	2.8	84
135	A rationally designed two-dimensional MoSe₂/Ti₂CO₂ heterojunction for photocatalytic overall water splitting: simultaneously suppressing electronâ€"hole recombination and photocorrosion. Chemical Science, 2021, 12, 2863-2869.	3.7	82
136	Electronic and Magnetic Properties of Metal Phthalocyanines on Au(111) Surface: A First-Principles Study. Journal of Physical Chemistry C, 2008, 112, 13650-13655.	1.5	81
137	Porous Boron Nitride with Tunable Pore Size. Journal of Physical Chemistry Letters, 2014, 5, 393-398.	2.1	81
138	Kernel Tuning and Nonuniform Influence on Optical and Electrochemical Gaps of Bimetal Nanoclusters. Journal of the American Chemical Society, 2018, 140, 3487-3490.	6.6	81
139	Modulating oxygen coverage of Ti3C2Tx MXenes to boost catalytic activity for HCOOH dehydrogenation. Nature Communications, 2020, 11, 4251.	5.8	81
140	Electronic and magnetic properties of V-doped anataseTiO2from first principles. Physical Review B, 2006, 74, .	1.1	80
141	Unusual Metallic Microporous Boron Nitride Networks. Journal of Physical Chemistry Letters, 2013, 4, 3484-3488.	2.1	80
142	Bipolar magnetic materials for electrical manipulation of spin-polarization orientation. Physical Chemistry Chemical Physics, 2013, 15, 15793.	1.3	78
143	Direct observation of single-molecule hydrogen-bond dynamics with single-bond resolution. Nature Communications, 2018, 9, 807.	5.8	78
144	Nonclassical Behavior in the Capacitance of a Nanojunction. Physical Review Letters, 2001, 86, 5321-5324.	2.9	77

#	Article	IF	Citations
145	Realizing Two-Dimensional Magnetic Semiconductors with Enhanced Curie Temperature by Antiaromatic Ring Based Organometallic Frameworks. Journal of the American Chemical Society, 2019, 141, 109-112.	6.6	77
146	Determining structural and chemical heterogeneities of surface species at the single-bond limit. Science, 2021, 371, 818-822.	6.0	77
147	Deformation-induced site selectivity for hydrogen adsorption on boron nitride nanotubes. Physical Review B, 2004, 69, .	1.1	75
148	Exploration of Structures of Two-Dimensional Boronâ€"Silicon Compounds with sp² Silicon. Journal of Physical Chemistry Letters, 2013, 4, 561-567.	2.1	75
149	Single-layer cadmium chalcogenides: promising visible-light driven photocatalysts for water splitting. Physical Chemistry Chemical Physics, 2016, 18, 17029-17036.	1.3	75
150	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
151	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
152	MAGNETISM IN GRAPHENE SYSTEMS. Nano, 2008, 03, 433-442.	0.5	70
153	Graphene Thickness Control via Gas-Phase Dynamics in Chemical Vapor Deposition. Journal of Physical Chemistry C, 2012, 116, 10557-10562.	1.5	70
154	Is Mayenite without Clathrated Oxygen an Inorganic Electride?. Angewandte Chemie - International Edition, 2004, 43, 6479-6482.	7.2	68
155	CO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>dissociation activated through electron attachment on the reduced rutile TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(110)-1<mml:math xmlns:mml="http://www.w3.org/1998	1.1	68
156	Electronic and magnetic structure of infinite-layer NdNiO2: trace of antiferromagnetic metal. Npj Quantum Materials, 2020, 5, .	1.8	66
157	Structural and electronic properties ofOsB2: A hard metallic material. Physical Review B, 2006, 74, .	1.1	65
158	Ï-Phosphorene: a new allotrope of phosphorene. Physical Chemistry Chemical Physics, 2017, 19, 2402-2408.	1.3	65
159	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
160	Formation energies of topological defects in carbon nanotubes. Physical Review B, 2000, 62, 12652-12655.	1.1	64
161	Transition metal atom embedded graphene for capturing CO: A first-principles study. International Journal of Hydrogen Energy, 2014, 39, 20190-20196.	3.8	62
162	Electrically Driven Single-Photon Superradiance from Molecular Chains in a Plasmonic Nanocavity. Physical Review Letters, 2019, 122, 233901.	2.9	62

#	Article	IF	Citations
163	What can a scanning tunneling microscope image do for the insulating alkanethiol molecules on Au(111) substrates?. Journal of Chemical Physics, 2002, 117, 851-856.	1.2	61
164	Evidence of van Hove Singularities in Ordered Grain Boundaries of Graphene. Physical Review Letters, 2014, 112, 226802.	2.9	61
165	Systematic Synthesis of Tellurium Nanostructures and Their Optical Properties: From Nanoparticles to Nanorods, Nanowires, and Nanotubes. ChemNanoMat, 2016, 2, 167-170.	1.5	61
166	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
167	Hydroxyls-induced oxygen activation on â€œinertâ€•Au nanoparticles for low-temperature CO oxidation. Journal of Catalysis, 2011, 277, 95-103.	3.1	59
168	Single- and few-layer BiOI as promising photocatalysts for solar water splitting. RSC Advances, 2017, 7, 24446-24452.	1.7	59
169	A class of Pb-free double perovskite halide semiconductors with intrinsic ferromagnetism, large spin splitting and high Curie temperature. Materials Horizons, 2018, 5, 961-968.	6.4	59
170	Fcc versus Nonâ€fcc Structural Isomerism of Gold Nanoparticles with Kernel Atom Packing Dependent Photoluminescence. Angewandte Chemie - International Edition, 2019, 58, 4510-4514.	7.2	59
171	Excited states of the 3d transition metal monoxides. Journal of Chemical Physics, 2003, 118, 9608-9613.	1.2	58
172	Iron-phthalocyanine molecular junction with high spin filter efficiency and negative differential resistance. Journal of Chemical Physics, 2012, 136, 064707.	1.2	58
173	Penta-Pt₂N₄: an ideal two-dimensional material for nanoelectronics. Nanoscale, 2018, 10, 16169-16177.	2.8	58
174	Gold atom-decorated CoSe₂nanobelts with engineered active sites for enhanced oxygen evolution. Journal of Materials Chemistry A, 2017, 5, 20202-20207.	5.2	57
175	A high performance catalyst for methane conversion to methanol: graphene supported single atom Co. Chemical Communications, 2018, 54, 2284-2287.	2.2	57
176	A Silver Nanocluster Containing Interstitial Sulfur and Unprecedented Chemical Bonds. Angewandte Chemie - International Edition, 2018, 57, 11273-11277.	7.2	57
177	Funnel hopping: Searching the cluster potential energy surface over the funnels. Journal of Chemical Physics, 2009, 130, 214112.	1.2	56
178	Structure sensitivity of low-temperature NO decomposition on Au surfaces. Journal of Catalysis, 2013, 304, 112-122.	3.1	56
179	Hydrogenated bilayer wurtzite SiC nanofilms: a two-dimensional bipolar magnetic semiconductor material. Physical Chemistry Chemical Physics, 2013, 15, 497-503.	1.3	55
180	Tunable Rashba spin splitting in Janus transition-metal dichalcogenide monolayers <i>via</i> charge doping. RSC Advances, 2020, 10, 6388-6394.	1.7	55

#	Article	IF	Citations
181	Average density of states in disordered graphene systems. Physical Review B, 2008, 77, .	1.1	54
182	Active hydrogen species on TiO2 for photocatalytic H2 production. Physical Chemistry Chemical Physics, 2014, 16, 7051.	1.3	54
183	Half-Metallicity in One-Dimensional Metal Trihydride Molecular Nanowires. Journal of the American Chemical Society, 2017, 139, 6290-6293.	6.6	54
184	Formation and diffusion of oxygen-vacancy pairs on TiO2(110)-(1Ã—1). Journal of Chemical Physics, 2008, 129, 044703.	1.2	52
185	Diamondization of chemically functionalized graphene and grapheneâ€“BN bilayers. Physical Chemistry Chemical Physics, 2012, 14, 8179.	1.3	52
186	Tuning Charge Transport in Aromaticâ€Ring Singleâ€Molecule Junctions via Ionicâ€Liquid Gating. Angewandte Chemie - International Edition, 2018, 57, 14026-14031.	7.2	52
187	First principles nuclear magnetic resonance signatures of graphene oxide. Journal of Chemical Physics, 2010, 133, 034502.	1.2	51
188	A many-body <i>GW</i>â€‰+â€‰BSE investigation of electronic and optical properties of C2N. Applied Physics Letters, 2016, 109, .	1.5	51
189	Structural Oscillation Revealed in Gold Nanoparticles. Journal of the American Chemical Society, 2020, 142, 12140-12145.	6.6	51
190	Interplay between hydrogen bonding and electron solvation on hydratedTiO2(110). Physical Review B, 2006, 73, .	1.1	50
191	Copper Nanocrystal Plane Effect on Stereoselectivity of Catalytic Deoxygenation of Aromatic Epoxides. Journal of the American Chemical Society, 2015, 137, 3791-3794.	6.6	50
192	Ultrafast Solid-State Transformation Pathway from New-Phased Goethite VOOH to Paramontroseite VO₂ to Rutile VO₂(R). Journal of Physical Chemistry C, 2011, 115, 791-799.	1.5	49
193	Superatomâ€“atom super-bonding in metallic clusters: a new look to the mystery of an Au₂₀ pyramid. Nanoscale, 2014, 6, 12440-12444.	2.8	49
194	A first-principles study of NO adsorption and oxidation on Au(111) surface. Journal of Chemical Physics, 2008, 129, 134708.	1.2	48
195	Highly Efficient Photothermal Effect by Atomic-Thickness Confinement in Two-Dimensional ZrNCl Nanosheets. ACS Nano, 2015, 9, 1683-1691.	7.3	48
196	Is the kernelâ€“staples match a keyâ€“lock match?. Chemical Science, 2018, 9, 2437-2442.	3.7	48
197	Construction of direct Zâ€Scheme photocatalysts for overall water splitting using twoâ€dimensional van der waals heterojunctions of metal dichalcogenides. Journal of Computational Chemistry, 2019, 40, 980-987.	1.5	48
198	Me-graphene: a graphene allotrope with near zero Poisson's ratio, sizeable band gap, and high carrier mobility. Nanoscale, 2020, 12, 19359-19366.	2.8	48

#	Article	IF	Citations
199	Calculated polarizabilities of small Si clusters. Physical Review A, 2000, 61, .	1.0	47
200	Lowâ€dimensional halfâ€metallic materials: theoretical simulations and design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1314.	6.2	47
201	<i>In-Situ</i> Generated High-Valent Iron Single-Atom Catalyst for Efficient Oxygen Evolution. Nano Letters, 2021, 21, 4795-4801.	4.5	47
202	Diamond as an inert substrate of graphene. Journal of Chemical Physics, 2013, 138, 054701.	1.2	46
203	Unveiling the full reaction path of the Suzukiâ€“Miyaura cross-coupling in a single-molecule junction. Nature Nanotechnology, 2021, 16, 1214-1223.	15.6	46
204	Nearly Free Electron Superatom States of Carbon and Boron Nitride Nanotubes. Nano Letters, 2010, 10, 4830-4838.	4.5	45
205	Surface Landau levels and spin states in bismuth (111) ultrathin films. Nature Communications, 2016, 7, 10814.	5.8	45
206	Kondo effect in single cobalt phthalocyanine molecules adsorbed on Au(111) monoatomic steps. Journal of Chemical Physics, 2008, 128, 234705.	1.2	44
207	Bilayer Graphene Growth via a Penetration Mechanism. Journal of Physical Chemistry C, 2014, 118, 6201-6206.	1.5	44
208	More accurate depiction of adsorption energy on transition metals using work function as one additional descriptor. Physical Chemistry Chemical Physics, 2017, 19, 12628-12632.	1.3	44
209	Photogenerated-Carrier Separation and Transfer in Two-Dimensional Janus Transition Metal Dichalcogenides and Graphene van der Waals Sandwich Heterojunction Photovoltaic Cells. Journal of Physical Chemistry Letters, 2020, 11, 4070-4079.	2.1	44
210	Efficient organometallic spin filter based on Europium-cyclooctatetraene wire. Journal of Chemical Physics, 2009, 131, .	1.2	43
211	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
212	A single-molecule electrical approach for amino acid detection and chirality recognition. Science Advances, 2021, 7, .	4.7	43
213	Geometric and electronic structure of aC60monolayer on Ag(100). Physical Review B, 2007, 75, .	1.1	42
214	Nitrogen-inserted nickel nanosheets with controlled orbital hybridization and strain fields for boosted hydrogen oxidation in alkaline electrolytes. Energy and Environmental Science, 2022, 15, 1234-1242.	15.6	42
215	Inorganic Electride:â€‰ Theoretical Study on Structural and Electronic Properties. Journal of the American Chemical Society, 2003, 125, 6050-6051.	6.6	41
216	Global Minimum Structures of Morse Clusters as a Function of the Range of the Potential:â€‰ 81 â‰ N â‰ 160. Journal of Physical Chemistry A, 2007, 111, 5287-5293.	1.1	41

#	ARTICLE	IF	CITATIONS
217	Magnetic states of zigzag graphene nanoribbons from first principles. Applied Physics Letters, 2009, 94, .	1.5	41
218	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
219	Proposal of a stable B₃S nanosheet as an efficient hydrogen evolution catalyst. Journal of Materials Chemistry A, 2019, 7, 3752-3756.	5.2	41
220	Electron-induced ferromagnetic ordering of Co-doped ZnO. Journal of Applied Physics, 2007, 102, 033915.	1.1	40
221	Electronic Stability of Phosphine-Protected Au₂₀ Nanocluster: Superatomic Bonding. Journal of Physical Chemistry C, 2013, 117, 13276-13282.	1.5	40
222	Electronic structure and aromaticity of large-scale hexagonal graphene nanoflakes. Journal of Chemical Physics, 2014, 141, 214704.	1.2	40
223	Density functional calculations of the polarizability and second-order hyperpolarizability ofC50Cl10. Physical Review A, 2005, 71, .	1.0	39
224	Ferrimagnetism in zigzag graphene nanoribbons induced by main-group adatoms. Applied Physics Letters, 2010, 96, .	1.5	39
225	Role of Surface Stress on the Reactivity of Anatase TiO₂(001). Journal of Physical Chemistry Letters, 2017, 8, 1764-1771.	2.1	39
226	Atomically thin semiconducting penta-PdP₂ and PdAs₂ with ultrahigh carrier mobility. Journal of Materials Chemistry C, 2018, 6, 9055-9059.	2.7	39
227	Toward Room-Temperature Magnetic Semiconductors in Two-Dimensional Ferrimagnetic Organometallic Lattices. Journal of Physical Chemistry Letters, 2019, 10, 2439-2444.	2.1	39
228	Effects Due to Interadsorbate Interactions on the Dipeptide/TiO2Surface Binding Mechanism Investigated by Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2007, 111, 7765-7771.	1.5	38
229	Half-Metallic Dirac Point in B-Edge Hydrogenated BN Nanoribbons. Journal of Physical Chemistry C, 2011, 115, 17252-17254.	1.5	38
230	Oxygen Vacancy-Controlled Reactivity of Hydroxyls on an FeO(111) Monolayer Film. Journal of Physical Chemistry C, 2011, 115, 6815-6824.	1.5	38
231	Understanding the Kondo resonance in the d-CoPc/Au(111) adsorption system. Journal of Chemical Physics, 2014, 141, 084713.	1.2	38
232	Rational Design of Two-dimensional Anode Materials: B₂S as a Strained Graphene. Journal of Physical Chemistry Letters, 2018, 9, 4852-4856.	2.1	38
233	Single Mo₁(W₁, Re₁) atoms anchored in pyrrolic-N₃doped graphene as efficient electrocatalysts for the nitrogen reduction reaction. Journal of Materials Chemistry A, 2021, 9, 6547-6554.	5.2	38
234	Two-Dimensional Giant Tunable Rashba Semiconductors with Two-Atom-Thick Buckled Honeycomb Structure. Nano Letters, 2021, 21, 740-746.	4.5	38

#	Article	IF	Citations
235	Low-cost alternatives to the Bethe-Salpeter equation: Towards simple hybrid functionals for excitonic effects in solids. Physical Review Research, 2020, 2, .	1.3	38
236	Environment-modulated Kondo phenomena in FePc/Au(111) adsorption systems. Physical Review B, 2016, 93, .	1.1	37
237	Coherent transport through spin-crossover magnet Fe₂complexes. Nanoscale, 2016, 8, 609-616.	2.8	37
238	Efficient Direct Band Gap Photovoltaic Material Predicted <i>Via</i> Doping Double Perovskites Cs₂AgBiX₆ (X = Cl, Br). Journal of Physical Chemistry C, 2021, 125, 10868-10875.	1.5	37
239	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
240	Comparative Study on Electronic Structures of Sc and Ti Contacts with Monolayer and Multilayer MoS₂. ACS Applied Materials & Interfaces, 2015, 7, 12981-12987.	4.0	36
241	Atomicâ€Level Insight into Optimizing the Hydrogen Evolution Pathway over a Co₁â€N₄ Singleâ€Site Photocatalyst. Angewandte Chemie, 2017, 129, 12359-12364.	1.6	36
242	Tuning Electronic Structure and Lattice Diffusion Barrier of Ternary Ptâ€"Inâ€"Ni for Both Improved Activity and Stability Properties in Oxygen Reduction Electrocatalysis. ACS Catalysis, 2019, 9, 11431-11437.	5.5	36
243	Improving the Activity of Electrocatalysts toward the Hydrogen Evolution Reaction, the Oxygen Evolution Reaction, and the Oxygen Reduction Reaction via Modification of Metal and Ligand of Conductive Two-Dimensional Metalâ€"Organic Frameworks. Journal of Physical Chemistry Letters, 2021, 12, 11652-11658.	2.1	36
244	Electronic structure of bilayer graphene: A real-space Greenâ€™s function study. Physical Review B, 2007, 75, .	1.1	35
245	Energy Level Realignment in Weakly Interacting Donorâ€"Acceptor Binary Molecular Networks. ACS Nano, 2014, 8, 1699-1707.	7.3	35
246	Light-Induced Type-II Band Inversion and Quantum Anomalous Hall State in Monolayer FeSe. Physical Review Letters, 2018, 120, 156406.	2.9	35
247	A new phase of the two-dimensional ReS₂ sheet with tunable magnetism. Journal of Materials Chemistry C, 2018, 6, 1248-1254.	2.7	35
248	Machine Learning K-Means Clustering Algorithm for Interpolative Separable Density Fitting to Accelerate Hybrid Functional Calculations with Numerical Atomic Orbitals. Journal of Physical Chemistry A, 2020, 124, 10066-10074.	1.1	35
249	Synthesis, Growth Mechanism, and Work Function at Highly Oriented {001} Surfaces of Bismuth Sulfide Microbelts. Journal of Physical Chemistry C, 2007, 111, 12145-12148.	1.5	34
250	Electronic structure of atomic Ti chains on semiconducting graphene nanoribbons: A first-principles study. Journal of Chemical Physics, 2007, 127, 164706.	1.2	34
251	<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
252	In-situ activated polycation as a multifunctional additive for Li-S batteries. Nano Energy, 2016, 26, 43-49.	8.2	34

#	ARTICLE	IF	CITATIONS
253	Probing intramolecular vibronic coupling through vibronic-state imaging. Nature Communications, 2021, 12, 1280.	5.8	34
254	Roomâ€Temperature Ferromagnetic Silver Vanadium Oxide (Ag_{1.2}V₃O₈): A Magnetic Semiconductor Nanoring Structure. Advanced Functional Materials, 2010, 20, 3666-3672.	7.8	33
255	Origin of the Ising ferrimagnetism and spin-charge coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LuFe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml: Physical Review B, 2009, 80, .	1.1	32
256	Synthesis and Properties Evolution of a Family of Tiara-like Phenylethanethiolated Palladium Nanoclusters. Scientific Reports, 2015, 5, 16628.	1.6	32
257	Double-hole codoped huge-gap semiconductor ZrO₂ for visible-light photocatalysis. Physical Chemistry Chemical Physics, 2016, 18, 17517-17524.	1.3	32
258	Strain-Stabilized Metastable Face-Centered Tetragonal Gold Overlayer for Efficient CO₂ Electroreduction. Nano Letters, 2021, 21, 1003-1010.	4.5	32
259	Organometallic Hexahapto-Functionalized Graphene: Band Gap Engineering with Minute Distortion to the Planar Structure. Journal of Physical Chemistry C, 2013, 117, 22156-22161.	1.5	31
260	Double aromaticity in transition metal centered double-ring boron clusters M@B2<i>n</i> (M = Ti, Cr,) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.2	31
261	[Ti₁₂In₆O₁₈(OOCC₆H₅)₃₀]: a multifunctional hetero-polyoxotitanate nanocluster with high stability and visible photoactivity. Dalton Transactions, 2017, 46, 678-684.	1.6	31
262	Interfacial Hydrogen-Bonding Dynamics in Surface-Facilitated Dehydrogenation of Water on TiO₂(110). Journal of the American Chemical Society, 2020, 142, 826-834.	6.6	31
263	Halogen modified two-dimensional covalent triazine frameworks as visible-light driven photocatalysts for overall water splitting. Science China Chemistry, 2020, 63, 1134-1141.	4.2	31
264	Electronic Structures of Defective Boron Nitride Nanotubes under Transverse Electric Fields. Journal of Physical Chemistry C, 2008, 112, 8424-8428.	1.5	30
265	Electrical control of carriers' spin orientation in the FeVTiSi Heusler alloy. Journal of Materials Chemistry C, 2015, 3, 2563-2567.	2.7	30
266	Point defects in lines in single crystalline phosphorene: directional migration and tunable band gaps. Nanoscale, 2016, 8, 17801-17808.	2.8	30
267	Atomic-level insights into strain effect on p-nitrophenol reduction via Au@Pd coreâ€“shell nanocubes as an ideal platform. Journal of Catalysis, 2020, 381, 427-433.	3.1	30
268	Two-Dimensional Multifunctional Metalâ€“Organic Frameworks with Simultaneous Ferro-/Ferrimagnetism and Vertical Ferroelectricity. Journal of Physical Chemistry Letters, 2020, 11, 4193-4197.	2.1	30
269	Geometric and Electronic Properties of Metallofullerene Fe@C60â€. Chinese Journal of Chemistry, 2006, 24, 1133-1136.	2.6	29
270	Band structure engineering of anatase TiO2 by metal-assisted P-O coupling. Journal of Chemical Physics, 2014, 140, 174705.	1.2	29

#	Article	IF	Citations
271	Goldâ€Doping of Doubleâ€Crown Pd Nanoclusters. Chemistry - A European Journal, 2017, 23, 18187-18192.	1.7	29
272	Graphdiyne as Hydrogen Purification Membrane. Chinese Journal of Chemical Physics, 2012, 25, 434-440.	0.6	28
273	The Nanoparticle Size Effect in Graphene Cutting: A â€œPacâ€Manâ€•Mechanism. Angewandte Chemie - International Edition, 2016, 55, 9918-9921.	7.2	28
274	Additive and Photochemical Manufacturing of Copper. Scientific Reports, 2016, 6, 39584.	1.6	28
275	Two-dimensional silicon crystals with sizable band gaps and ultrahigh carrier mobility. Nanoscale, 2018, 10, 1265-1271.	2.8	28
276	Î²-SnS/GaSe heterostructure: a promising solar-driven photocatalyst with low carrier recombination for overall water splitting. Journal of Materials Chemistry A, 2022, 10, 3443-3453.	5.2	28
277	Effects of discrete energy levels on single-electron tunneling in coupled metal particles. Applied Physics Letters, 2003, 82, 3767-3769.	1.5	27
278	Density functional theory study of Wn (n=2â€“4) clusters. Computational and Theoretical Chemistry, 2005, 757, 113-118.	1.5	27
279	Spin-unrestricted linear-scaling electronic structure theory and its application to magnetic carbon-doped boron nitride nanotubes. Journal of Chemical Physics, 2005, 123, 124105.	1.2	27
280	Negative differential resistance devices by using N-doped graphene nanoribbons. Journal of Chemical Physics, 2014, 140, 164703.	1.2	27
281	Density Functional Study of Nonlinear Optical Properties of Grossly Warped Nanographene C₈₀H₃₀. Journal of Physical Chemistry C, 2014, 118, 3313-3318.	1.5	27
282	Atomistic Simulations of Graphene Growth: From Kinetics to Mechanism. Accounts of Chemical Research, 2018, 51, 728-735.	7.6	27
283	Water Confined in Nanocapillaries: Two-Dimensional Bilayer Squarelike Ice and Associated Solidâ€“Liquidâ€“Solid Transition. Journal of Physical Chemistry C, 2018, 122, 6704-6712.	1.5	27
284	Ambipolar Half-Metallicity in One-Dimensional Metalâ€“(1,2,4,5-Benzenetetramine) Coordination Polymers via Carrier Doping. Journal of Physical Chemistry C, 2018, 122, 989-994.	1.5	27
285	Largeâ€Spinâ€Gap Nodalâ€Line Halfâ€Metal and Highâ€Temperature Ferromagnetic Semiconductor in Cr₂X₃ (X=O,S,Se) Monolayers. Advanced Electronic Materials, 2020, 6, 1900490.	2.6	27
286	Simulating Periodic Systems on a Quantum Computer Using Molecular Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 6904-6914.	2.3	27
287	A theoretical study of small copper oxide clusters: Cu2Ox (x=1â€“4). Journal of Chemical Physics, 2004, 120, 2746-2751.	1.2	26
288	A first principles study on organic molecule encapsulated boron nitride nanotubes. Journal of Chemical Physics, 2008, 128, 164701.	1.2	26

#	Article	IF	Citations
289	STM tip-assisted single molecule chemistry. Physical Chemistry Chemical Physics, 2013, 15, 12428.	1.3	26
290	SiN-SiC nanofilm: A nano-functional ceramic with bipolar magnetic semiconducting character. Applied Physics Letters, 2014, 104, .	1.5	26
291	Two-dimensional interlocked pentagonal bilayer ice: how do water molecules form a hydrogen bonding network?. Physical Chemistry Chemical Physics, 2016, 18, 14216-14221.	1.3	26
292	Kernel Homology in Gold Nanoclusters. Angewandte Chemie - International Edition, 2018, 57, 15450-15454.	7.2	26
293	Room-Temperature Ferromagnetism in Transition Metal Embedded Borophene Nanosheets. Journal of Physical Chemistry Letters, 2019, 10, 4417-4421.	2.1	26
294	High-Throughput Screening of Rattling-Induced Ultralow Lattice Thermal Conductivity in Semiconductors. Journal of the American Chemical Society, 2022, 144, 4448-4456.	6.6	26
295	Modified Morse potential for unification of the pair interactions. Journal of Chemical Physics, 2007, 127, 124104.	1.2	25
296	Enhanced photoelectrochemical performance of anatase TiO₂ for water splitting via surface codoping. RSC Advances, 2017, 7, 39877-39884.	1.7	25
297	Room-temperature magnetism and tunable energy gaps in edge-passivated zigzag graphene quantum dots. Npj 2D Materials and Applications, 2019, 3, .	3.9	25
298	Direct bandgap engineering with local biaxial strain in few-layer MoS2 bubbles. Nano Research, 2020, 13, 2072-2078.	5.8	25
299	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
300	Two-dimensional bipolar magnetic semiconductors with high Curie-temperature and electrically controllable spin polarization realized in exfoliated Cr(pyrazine)2 monolayers. Science China Chemistry, 2021, 64, 2212-2217.	4.2	25
301	Enhanced Curie Temperature of Two-Dimensional Cr(II) Aromatic Heterocyclic Metalâ€“Organic Framework Magnets via Strengthened Orbital Hybridization. Nano Letters, 2022, 22, 1573-1579.	4.5	25
302	Dual-metal atoms embedded into two-dimensional covalent organic framework as efficient electrocatalysts for oxygen evolution reaction: A DFT study. Nano Research, 2022, 15, 7994-8000.	5.8	25
303	The B3LYP hybrid density functional study on solids. Frontiers of Physics in China, 2006, 1, 339-343.	1.0	24
304	Electronic, Magnetic, and Transport Properties of Fe-COT Clusters: A Theoretical Study. Journal of Physical Chemistry C, 2010, 114, 11946-11950.	1.5	24
305	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
306	Diffusion and desorption of oxygen atoms on graphene. Journal of Physics Condensed Matter, 2013, 25, 405301.	0.7	24

#	Article	IF	Citations
307	Electron-phonon interaction in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ca</mml:mi><mml:mn>2</mml:mn></mm… mathvariant="normal">N</mml:mi></mml:mrow></mml:math> monolayer: Intrinsic mobility of electrene. Physical Review B, 2018, 98, .	1.1	24
308	A Silver Nanocluster Containing Interstitial Sulfur and Unprecedented Chemical Bonds. Angewandte Chemie, 2018, 130, 11443-11447.	1.6	24
309	Tunable Schottky and Ohmic contacts in graphene and tellurene van der Waals heterostructures. Physical Chemistry Chemical Physics, 2019, 21, 23611-23619.	1.3	24
310	Doping dependence of electronic structure of infinite-layer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>NdNiO</mml:mi></mml:mrow><mml:mn>2… Physical Review B, 2021, 103, .	1.1	24
311	Linear scaling electronic structure calculations with numerical atomic basis set. International Reviews in Physical Chemistry, 2010, 29, 665-691.	0.9	23
312	A theoretical study of spin-polarized transport properties of planar four-coordinate Fe complexes. Chemical Physics Letters, 2012, 539-540, 102-106.	1.2	23
313	Proposal of a general scheme to obtain room-temperature spin polarization in asymmetric antiferromagnetic semiconductors. Physical Review B, 2015, 92, .	1.1	23
314	Tetrahedral Au₁₇⁺: A Superatomic Molecule with a Au₁₃ FCC Core. Journal of Physical Chemistry C, 2015, 119, 23274-23278.	1.5	23
315	Azide Passivation of Black Phosphorus Nanosheets: Covalent Functionalization Affords Ambient Stability Enhancement. Angewandte Chemie, 2019, 131, 1493-1497.	1.6	23
316	Accelerating Excitation Energy Computation in Molecules and Solids within Linear-Response Time-Dependent Density Functional Theory via Interpolative Separable Density Fitting Decomposition. Journal of Chemical Theory and Computation, 2020, 16, 964-973.	2.3	23
317	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
318	Electric-Field Tunable Magnetism in van der Waals Bilayers with A-Type Antiferromagnetic Order: Unipolar versus Bipolar Magnetic Semiconductor. Nano Letters, 2021, 21, 7050-7055.	4.5	23
319	Controlling the Valenceâ€Electron Arrangement of Nickel Active Centers for Efficient Hydrogen Oxidation Electrocatalysis. Angewandte Chemie - International Edition, 2022, 61, .	7.2	23
320	Structure dependent quantum confinement effect in hydrogen-terminated nanodiamond clusters. Journal of Applied Physics, 2010, 108, 094303.	1.1	22
321	Highly entangled K0.5V2O5 superlong nanobelt membranes for flexible nonvolatile memory devices. Journal of Materials Chemistry, 2012, 22, 18214.	6.7	22
322	Metal-Free Magnetism and Half-Metallicity of Carbon Nitride Nanotubes: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 22491-22498.	1.5	22
323	Anatase TiO2 codoping with sulfur and acceptor IIB metals for water splitting. International Journal of Hydrogen Energy, 2016, 41, 13050-13057.	3.8	22
324	Proximity Effect Induced Spin Injection in Phosphorene on Magnetic Insulator. ACS Applied Materials & Interfaces, 2017, 9, 38999-39010.	4.0	22

#	Article	IF	Citations
325	Tuning Charge Transport in Aromaticâ€Ring Singleâ€Molecule Junctions via Ionicâ€Liquid Gating. Angewandte Chemie, 2018, 130, 14222-14227.	1.6	22
326	Computation-Guided Development of Platinum Alloy Catalyst for Carbon Monoxide Preferential Oxidation. ACS Catalysis, 2018, 8, 5777-5786.	5.5	22
327	Tunable Rashba Spin Splitting in Two-Dimensional Polar Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 1932-1939.	2.1	22
328	Single-molecule field effect and conductance switching driven by electric field and proton transfer. Science Advances, 2022, 8, eabm3541.	4.7	22
329	Spinâ€“Orbit Coupling in 2D Semiconductors: A Theoretical Perspective. Journal of Physical Chemistry Letters, 2021, 12, 12256-12268.	2.1	22
330	Theoretical studies of neutral and cationic selenium clusters. Physical Review B, 2000, 62, 17026-17030.	1.1	21
331	Mechanism for tautomerization induced conductance switching of naphthalocyanin molecule. Applied Physics Letters, 2009, 95, 182103.	1.5	21
332	Controlling Electronic States and Transport Properties at the Level of Single Molecules. Advanced Materials, 2010, 22, 1967-1971.	11.1	21
333	Methanol-Selective Oxidation Pathways on Au Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2014, 118, 17511-17520.	1.5	21
334	A Density Functional Study of the Nonlinear Optical Properties of Edgeâ€Functionalized Nonplanar Nanographenes. ChemPhysChem, 2015, 16, 2783-2788.	1.0	21
335	Kondo screening and spin excitation in few-layer CoPc molecular assembly stacking on Pb(111) surface: A DFT+HEOM study. Journal of Chemical Physics, 2016, 145, 154301.	1.2	21
336	Water on silicene: A hydrogen bond-autocatalyzed physisorptionâ€“chemisorptionâ€“dissociation transition. Nano Research, 2017, 10, 2223-2233.	5.8	21
337	Pressure-induced organic topological nodal-line semimetal in the three-dimensional molecular crystal Pd(dddt)2. Physical Review B, 2018, 97, .	1.1	21
338	Revealing Chargeâ€•and Temperatureâ€Dependent Movement Dynamics and Mechanism of Individual Molecular Machines. Small Methods, 2019, 3, 1900464.	4.6	21
339	Realizing CsPbBr₃ Light-Emitting Diode Arrays Based on PDMS Template Confined Solution Growth of Single-Crystalline Perovskite. Journal of Physical Chemistry Letters, 2020, 11, 8275-8282.	2.1	21
340	Designing Direct Z-Scheme Heterojunctions Enabled by Edge-Modified Phosphorene Nanoribbons for Photocatalytic Overall Water Splitting. Journal of Physical Chemistry Letters, 2022, 13, 1-11.	2.1	21
341	A theoretical study of the linear OCuO species. Journal of Chemical Physics, 1999, 111, 1477-1482.	1.2	20
342	Distinct molecule adsorption behaviors on warped nanographene C80H30: A theoretical study. Carbon, 2016, 100, 428-434.	5.4	20

#	Article	IF	Citations
343	Stable Heteropolyoxotitanate Nanocluster for Full Solar Spectrum Photocatalytic Hydrogen Evolution. Journal of Physical Chemistry C, 2017, 121, 18326-18332.	1.5	20
344	Room temperature electrofreezing of water yields a missing dense ice phase in the phase diagram. Nature Communications, 2019, 10, 1925.	5.8	20
345	Thgraphene: a novel two-dimensional carbon allotrope as a potential multifunctional material for electrochemical water splitting and potassium-ion batteries. Journal of Materials Chemistry A, 2022, 10, 9848-9857.	5.2	20
346	A theoretical study of the CuO3 species. Journal of Chemical Physics, 2000, 113, 7867-7873.	1.2	19
347	Thermal Stabilities of the Microhydrated Zwitterionic Glycine: A Kinetics and Dynamics Study. Journal of Physical Chemistry A, 2009, 113, 480-483.	1.1	19
348	Implementation of Exact Exchange with Numerical Atomic Orbitals. Journal of Physical Chemistry A, 2010, 114, 1039-1043.	1.1	19
349	Accurate Determination of the Quasiparticle and Scaling Properties Surrounding the Quantum Critical Point of Disordered Three-Dimensional Dirac Semimetals. Physical Review Letters, 2017, 118, 146401.	2.9	19
350	The Contacts of the Monolayer Semiconductor C₂N with 2D Metal Electrodes. Advanced Theory and Simulations, 2019, 2, 1800161.	1.3	19
351	Thickness Dependent Magnetic Transition in Few Layer 1T Phase CrTe₂. Journal of Physical Chemistry Letters, 2021, 12, 6847-6851.	2.1	19
352	Molecular molds for regularizing Kondo states at atom/metal interfaces. Nature Communications, 2020, 11, 2566.	5.8	19
353	A review of bipolar magnetic semiconductors from theoretical aspects. Fundamental Research, 2022, 2, 511-521.	1.6	19
354	Wavelike electronic energy transfer in donorâ€"acceptor molecular systems through quantum coherence. Nature Nanotechnology, 2022, 17, 729-736.	15.6	19
355	Electronic transport in Z-junction carbon nanotubes. Journal of Chemical Physics, 2004, 120, 7733-7737.	1.2	18
356	Nano-scale displacement sensing based on van der Waals interactions. Nanoscale, 2015, 7, 8962-8967.	2.8	18
357	Manipulation of spin and magnetic anisotropy in bilayer magnetic molecular junctions. Physical Chemistry Chemical Physics, 2018, 20, 26396-26404.	1.3	18
358	Interpolative Separable Density Fitting Decomposition for Accelerating Hartreeâ€"Fock Exchange Calculations within Numerical Atomic Orbitals. Journal of Physical Chemistry A, 2020, 124, 5664-5674.	1.1	18
359	Raman Detection of Bond Breaking and Making of a Chemisorbed Up-Standing Single Molecule at Single-Bond Level. Journal of Physical Chemistry Letters, 2021, 12, 1961-1968.	2.1	18
360	Steric Hindrance Effect in High-Temperature Reactions. CCS Chemistry, 2020, 2, 460-467.	4.6	18

#	Article	IF	Citations
361	Controllable p and n doping of single-walled carbon nanotubes by encapsulation of organic molecules and fullerene: A theoretical investigation. Applied Physics Letters, 2005, 86, 223113.	1.5	17
362	Linear-Scaling Density Matrix Perturbation Treatment of Electric Fields in Solids. Physical Review Letters, 2006, 97, 266402.	2.9	17
363	Electronic structures of organic molecule encapsulated BN nanotubes under transverse electric field. Journal of Chemical Physics, 2008, 129, 024710.	1.2	17
364	Surface and size effects on the charge state of NV center in nanodiamonds. Computational and Theoretical Chemistry, 2013, 1021, 49-53.	1.1	17
365	Control of spin in a La(Mn,Zn)AsO alloy by carrier doping. Journal of Materials Chemistry C, 2013, 1, 7197.	2.7	17
366	Electronic and optical properties of TiO2 nanotubes and arrays: a first-principles study. Physical Chemistry Chemical Physics, 2014, 16, 11519.	1.3	17
367	Formation of bilayer clathrate hydrates. Journal of Materials Chemistry A, 2015, 3, 5547-5555.	5.2	17
368	Photochemical Copper Coating on 3D Printed Thermoplastics. Scientific Reports, 2016, 6, 31188.	1.6	17
369	Spin switch in iron phthalocyanine on Au(111) surface by hydrogen adsorption. Journal of Chemical Physics, 2017, 147, 134701.	1.2	17
370	The roles of buckled geometry and water environment in the excitonic properties of graphitic C₃N₄. Nanoscale, 2018, 10, 3738-3743.	2.8	17
371	Visualizing Elementary Reactions of Methanol by Electrons and Holes on TiO₂(110) Surface. Journal of Physical Chemistry C, 2018, 122, 28805-28814.	1.5	17
372	Electronic and magnetic properties of CoPc and FePc molecules on graphene: the substrate, defect, and hydrogen adsorption effects. Physical Chemistry Chemical Physics, 2019, 21, 5424-5434.	1.3	17
373	Module Replacement of Gold Nanoparticles by a Pseudo-AGR Process. Acta Chimica Sinica, 2020, 78, 407.	0.5	17
374	Low-Rank Approximations Accelerated Plane-Wave Hybrid Functional Calculations with k-Point Sampling. Journal of Chemical Theory and Computation, 2022, 18, 206-218.	2.3	17
375	Molecular Design of Two-Dimensional Covalent Heptazine Frameworks for Photocatalytic Overall Water Splitting under Visible Light. Journal of Physical Chemistry Letters, 2022, 13, 3949-3956.	2.1	17
376	A theoretical study of the NiO2 species. Journal of Chemical Physics, 2003, 118, 6868-6873.	1.2	16
377	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
378	High performance computing of DGDFT for tens of thousands of atoms using millions of cores on Sunway TaihuLight. Science Bulletin, 2021, 66, 111-119.	4.3	16

#	Article	IF	Citations
379	C₇N₆/Sc₂CCl₂ Weak van der Waals Heterostructure: A Promising Visible-Light-Driven <i>Z</i>-Scheme Water Splitting Photocatalyst with Interface Ultrafast Carrier Recombination. Journal of Physical Chemistry Letters, 2022, 13, 1473-1479.	2.1	16
380	Nearly Free Electron State in Graphane Nanoribbon Superlattice. Chinese Journal of Chemical Physics, 2011, 24, 22-24.	0.6	15
381	Efficient spin filter based on FeN₄complexes between carbon nanotube electrodes. Nanotechnology, 2012, 23, 255202.	1.3	15
382	Transport spin polarization of magnetic C28 molecular junctions. Chemical Physics Letters, 2012, 535, 111-115.	1.2	15
383	New insights into the stability and structural evolution of some gold nanoclusters. Nanoscale, 2017, 9, 856-861.	2.8	15
384	Spin-Crossover and Coherent Transport Behaviors of a Six-Coordinate Iron(II) Complex with a N₄O₂ Donor Set. Journal of Physical Chemistry C, 2019, 123, 16366-16372.	1.5	15
385	Tunable n-type and p-type doping of two-dimensional layered PdSe₂<i>via</i> organic molecular adsorption. Physical Chemistry Chemical Physics, 2020, 22, 12973-12979.	1.3	15
386	Efficient interlayer charge release for high-performance layered thermoelectrics. National Science Review, 2021, 8, nwaa085.	4.6	15
387	Detecting a Moleculeâˆ’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
388	Coherent interference in the resonant dissociative electron attachment to carbon monoxide. Physical Review A, 2013, 88, .	1.0	14
389	A computational infrared spectroscopic study of graphene oxide. Journal of Chemical Physics, 2013, 139, 084704.	1.2	14
390	First principles study of fluorine substitution on two-dimensional germanane. Journal of Physics Condensed Matter, 2014, 26, 335302.	0.7	14
391	Nonnuclear Nearly Free Electron Conduction Channels Induced by Doping Charge in Nanotubeâ€“Molecular Sheet Composites. Journal of Physical Chemistry A, 2014, 118, 7255-7260.	1.1	14
392	Nano-scale polarâ€“nonpolar oxide heterostructures for photocatalysis. Nanoscale, 2016, 8, 6057-6063.	2.8	14
393	Ion Conductivity Enhancement in Antiâ€Spinel Li₃OBr with Intrinsic Vacancies. Advanced Theory and Simulations, 2019, 2, 1800138.	1.3	14
394	The Synthesis of Chiral Ag 4 Pd 2 (SR) 8 by Nonreplaced Galvanic Reaction. Particle and Particle Systems Characterization, 2019, 36, 1900003.	1.2	14
395	Nodal-loop half metallicity in a two-dimensional Fe₄N₂ pentagon crystal with room-temperature ferromagnetism. Nanoscale, 2021, 13, 19493-19499.	2.8	14
396	High Curie Temperature and Intrinsic Ferromagnetic Half-Metallicity in Mn₂X₃ (X = S, Se, Te) Nanosheets. Journal of Physical Chemistry Letters, 2021, 12, 11790-11794.	2.1	14

#	Article	IF	Citations
397	Electronic transport properties ofPdâ€Hjunctions between twoPdHx(x=0,0.25,0.5,0.75,1)electrodes: A nonequilibrium Greenâ€™s function study. Physical Review B, 2005, 72, .	1.1	13
398	Linear scaling calculation of band edge states and doped semiconductors. Journal of Chemical Physics, 2007, 126, 244707.	1.2	13
399	Ab initio photoionization dynamics of Î²-alanine. Journal of Chemical Physics, 2007, 126, 141103.	1.2	13
400	First-Principles Study of Molecular Clusters Formed by Nitric Acid and Ammonia. Journal of Physical Chemistry A, 2017, 121, 661-668.	1.1	13
401	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
402	Realizing Effective Cubic-Scaling Coulomb Hole Plus Screened Exchange Approximation in Periodic Systems via Interpolative Separable Density Fitting with a Plane-Wave Basis Set. Journal of Physical Chemistry A, 2021, 125, 7545-7557.	1.1	13
403	High-resolution scanning tunneling microscopy for molecules. Ultramicroscopy, 2004, 98, 317-334.	0.8	12
404	Linear scaling calculation of maximally localized Wannier functions with atomic basis set. Journal of Chemical Physics, 2006, 124, 234108.	1.2	12
405	Are Azafullerene Encapsulated Single-Walled Carbon Nanotubes n-Type Semiconductors?. Journal of Physical Chemistry C, 2011, 115, 12760-12762.	1.5	12
406	Porous germanene as a highly efficient gas separation membrane. Nanoscale, 2017, 9, 17505-17512.	2.8	12
407	First-Principles Study on Layered C₂Nâ€“Metal Interfaces. Langmuir, 2018, 34, 2647-2653.	1.6	12
408	An efficient nanocluster catalyst for Sonogashira reaction. Journal of Catalysis, 2021, 401, 206-213.	3.1	12
409	Schottky and Ohmic Contacts at Î±-Tellurene/2D Metal Interfaces. ACS Applied Electronic Materials, 2022, 4, 1082-1088.	2.0	12
410	Electrical rectification by selective wave-function coupling in small Ag clusters on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Si</mml:mtext><mml:mrow><mml:mo>(</mml:mo><mml:mrow><mml:mn>111</mml:mn> Physical Review B, 2010, 81, .	1.1	11
411	Important Structural Factors Controlling the Conductance of DNA Pairs in Molecular Junctions. Journal of Physical Chemistry C, 2010, 114, 14240-14242.	1.5	11
412	Understanding the concept of randomness in inelastic electron tunneling excitations. Physical Chemistry Chemical Physics, 2010, 12, 12012.	1.3	11
413	Theoretical investigation of gold based model catalysts. Science China Chemistry, 2015, 58, 565-573.	4.2	11
414	On the shuttling mechanism of a chlorine atom in a chloroaluminum phthalocyanine based molecular switch. Physical Chemistry Chemical Physics, 2017, 19, 22401-22405.	1.3	11

#	Article	IF	Citations
415	Significantly enhanced magnetoresistance in monolayer WTe2via heterojunction engineering: a first-principles study. Nanoscale, 2018, 10, 22231-22236.	2.8	11
416	Control of highly anisotropic electrical conductance of tellurene by strain-engineering. Nanoscale, 2019, 11, 21775-21781.	2.8	11
417	Designing Two-Dimensional Versatile Room-Temperature Ferromagnets via Assembling Large-Scale Magnetic Quantum Dots. Nano Letters, 2021, 21, 9816-9823.	4.5	11
418	A theoretical study of the Y $mathsf{_{3}}$ O clusters. European Physical Journal D, 2004, 29, 27-31.	0.6	10
419	STM studies of single molecules: molecular orbital aspects. Chemical Communications, 2011, 47, 2747.	2.2	10
420	Reply to â€œComment on â€˜Two-Dimensional Boron Monolayer Sheetsâ€™â€. ACS Nano, 2013, 7, 880-881.	7.3	10
421	Orbital-selective single molecule rectifier on graphene-covered Ru(0001) surface. Applied Physics Letters, 2013, 102, 163506.	1.5	10
422	Enhanced selective oxidation of h-BN nanosheet through a substrate-mediated localized charge effect. Physical Chemistry Chemical Physics, 2017, 19, 4435-4439.	1.3	10
423	A short review of nanographenes: structures, properties and applications. Molecular Physics, 2018, 116, 987-1002.	0.8	10
424	Single Pt atoms supported on oxidized graphene as a promising catalyst for hydrolysis of ammonia borane. Chinese Journal of Chemical Physics, 2018, 31, 641-648.	0.6	10
425	Kernel Homology in Gold Nanoclusters. Angewandte Chemie, 2018, 130, 15676-15680.	1.6	10
426	Two-level iterative solver for linear response time-dependent density functional theory with plane wave basis set. Journal of Chemical Physics, 2021, 154, 064101.	1.2	10
427	Quantum algorithms for electronic structures: basis sets and boundary conditions. Chemical Society Reviews, 2022, 51, 3263-3279.	18.7	10
428	Insights into the effect of substrate adsorption behavior over heme-like Fe1/AC single-atom catalyst. Nano Research, 2022, 15, 5970-5976.	5.8	10
429	Bamboolike carbon nitride nanotubes (C9N5H3): Atomic-scale construction, synthesis and lithium battery applications. Applied Physics Letters, 2007, 90, 113116.	1.5	9
430	Orientation-sensitive nonlinear growth of graphene: An epitaxial growth mechanism determined by geometry. Physical Review B, 2013, 88, .	1.1	9
431	The stabilization of the rocksalt structured tantalum nitride. Journal of Applied Physics, 2017, 122, .	1.1	9
432	Significantly Enhanced Charge Separation in Rippled Monolayer Graphitic C 3 N 4. ChemCatChem, 2019, 11, 6252-6257.	1.8	9

#	Article	IF	Citations
433	Fcc versus Nonâ€fcc Structural Isomerism of Gold Nanoparticles with Kernel Atom Packing Dependent Photoluminescence. Angewandte Chemie, 2019, 131, 4558-4562.	1.6	9
434	Formation of Plasmonic Polarons in Highly Electron-Doped Anatase TiO2. Nano Letters, 2021, 21, 430-436.	4.5	9
435	Electrochemistry of Pâ€“C Bonds in Phosphorusâ€“Carbon Based Anode Materials. ACS Applied Materials & Interfaces, 2022, 14, 18506-18512.	4.0	9
436	Bipolar Magnetic Molecules for Spinâ€Polarized Electric Current in Molecular Junctions. Angewandte Chemie - International Edition, 2022, 61, .	7.2	9
437	KSSOLV 2.0: An efficient MATLAB toolbox for solving the Kohn-Sham equations with plane-wave basis set. Computer Physics Communications, 2022, 279, 108424.	3.0	9
438	A first-principles study of acetylene and its evolution products on Cu(001). Journal of Chemical Physics, 2002, 116, 3104-3108.	1.2	8
439	DENSITY FUNCTIONAL THEORY STUDY OF W5 CLUSTERS. International Journal of Modern Physics B, 2005, 19, 2427-2432.	1.0	8
440	Quantum Dot Based on Z-shaped Graphene Nanoribbon: First-principles Study. Chinese Journal of Chemical Physics, 2007, 20, 489-494.	0.6	8
441	First-principles Study of Geometric and Electronic Structures of Si(111)-âˆš7ÂÃ—Ââˆš3-In Surface Reconstruction. Chinese Journal of Chemical Physics, 2012, 25, 403-408.	0.6	8
442	The Nanoparticle Size Effect in Graphene Cutting: A â€œPacâ€Manâ€• Mechanism. Angewandte Chemie, 2016, 128, 10072-10075.	1.6	8
443	Quantum stability and magic lengths of metal atom wires. Physical Review B, 2016, 93, .	1.1	8
444	Highly efficient heterojunction solar cells enabled by edge-modified tellurene nanoribbons. Physical Chemistry Chemical Physics, 2020, 22, 28414-28422.	1.3	8
445	The dynamic parallel distribution algorithm for hybrid density-functional calculations in HONPAS package. Computer Physics Communications, 2020, 254, 107204.	3.0	8
446	Are pyridinium ylides radicals?. Chemical Communications, 2020, 56, 11287-11290.	2.2	8
447	Theoretical Study on Geometrical and Electronic Properties of Anionic and Neutral V2O6 Clusters. Chinese Journal of Chemical Physics, 2006, 19, 391-394.	0.6	7
448	Protonation effects on electron transport through diblock molecular junctions: A theoretical study. Science in China Series B: Chemistry, 2008, 51, 1159-1165.	0.8	7
449	Density functional study on mechanism of CO oxidation with activated water on O/Au (111) surface. Science Bulletin, 2009, 54, 1973-1977.	4.3	7
450	Carrier-tunable magnetism of graphene with single-atom vacancy. Journal of Applied Physics, 2013, 113, 213709.	1.1	7

#	ARTICLE	IF	CITATIONS
451	Electronic structure engineering in chemically modified ultrathin ZnO nanofilms via a built-in heterointerface. RSC Advances, 2014, 4, 18718-18723.	1.7	7
452	Efficient Method for Fast Simulation of Scanning Tunneling Microscopy with a Tip Effect. Journal of Physical Chemistry A, 2014, 118, 8953-8959.	1.1	7
453	Three-Dimensional Covalently Linked Allotropic Structures of Phosphorus. Journal of Physical Chemistry C, 2016, 120, 26453-26458.	1.5	7
454	Surface alloy engineering in 2D trigonal lattice: giant Rashba spin splitting and two large topological gaps. New Journal of Physics, 2018, 20, 023041.	1.2	7
455	Two-dimensional transitional metal dihydride crystals with anisotropic and spin-polarized Fermi Dirac cones. Journal of Materials Chemistry C, 2018, 6, 11243-11247.	2.7	7
456	Computational Design of Oneâ€Dimensional Ferromagnetic Semiconductors in Transition Metal Embedded Stannaspherene Nanowires. Chinese Journal of Chemistry, 2019, 37, 1021-1024.	2.6	7
457	Precise Spin Manipulation of Single Molecule Positioning on Graphene by Coordination Chemistry. Journal of Physical Chemistry Letters, 2020, 11, 9819-9827.	2.1	7
458	Creation of the Dirac Nodal Line by Extrinsic Symmetry Engineering. Nano Letters, 2020, 20, 2157-2162.	4.5	7
459	Assessment of the Mass Factor for the Electronâ€“Phonon Coupling in Solids. Journal of Physical Chemistry C, 2021, 125, 6479-6485.	1.5	7
460	Orbital Design of Two-Dimensional Transition-Metal Peroxide Kagome Crystals with Anionogenic Dirac Half-Metallicity. Journal of Physical Chemistry Letters, 2021, 12, 3528-3534.	2.1	7
461	Low-threshold amplification of spontaneous emission from AgInS₂ quantum dots. Journal of Materials Chemistry C, 2020, 8, 8515-8520.	2.7	7
462	Theoretical design of two-dimensional visible light-driven photocatalysts for overall water splitting. Chemical Physics Reviews, 2022, 3, .	2.6	7
463	Promoting Water Activation by Photogenerated Holes in Monolayer C₂N. Journal of Physical Chemistry Letters, 2022, 13, 3332-3337.	2.1	7
464	Reducing Circuit Depth in Adaptive Variational Quantum Algorithms via Effective Hamiltonian Theories. Journal of Chemical Theory and Computation, 2022, 18, 4795-4805.	2.3	7
465	AFM study of crystalline cellulose in the cell walls of straw. Polymer International, 2006, 55, 87-92.	1.6	6
466	Atomic and Molecular Chemisorption of Oxygen in WO4 Clusters. Chinese Journal of Chemical Physics, 2007, 20, 78-82.	0.6	6
467	Nondecaying long range effect of surface decoration on the charge state of NV center in diamond. Journal of Chemical Physics, 2013, 138, 034702.	1.2	6
468	Transition between direct gap and indirect gap in two dimensional hydrogenated honeycomb Si x Ge1âˆ'x alloys. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	6

#	Article	IF	Citations
469	SP3-Hybridization Feature of Ag4 Superatom in Superatomic Molecules. Chinese Journal of Chemical Physics, 2015, 28, 476-480.	0.6	6
470	Coronoid nanographene C216 as hydrogen purification membrane: A density functional theory study. Carbon, 2018, 135, 112-117.	5.4	6
471	Spin-flip excitations induced by dehydrogenation in a magnetic single-molecule junction. Journal of Chemical Physics, 2019, 151, 224704.	1.2	6
472	Efficient parallel linear scaling method to get the response density matrix in all-electron real-space density-functional perturbation theory. Computer Physics Communications, 2021, 258, 107613.	3.0	6
473	First-Principles Calculations of Room-Temperature Antiferromagnetism in Crystalline Transition-Metal Borate Nanosheets: Implications for Spintronics Applications. ACS Applied Nano Materials, 2021, 4, 10877-10885.	2.4	6
474	Two-Dimensional Multifunctional Metalâ€“Organic Framework with Intrinsic Bipolar Magnetic Semiconductivity and Negative Poissonâ€™s Ratio. ACS Applied Electronic Materials, 2022, 4, 3198-3204.	2.0	6
475	Electron-Induced Synthesis of Dimethyl Ether in the Liquidâ€“Vapor Interface of Methanol. Journal of Physical Chemistry Letters, 0, , 5220-5225.	2.1	6
476	Identifying Photocatalytic Active Sites of C₂H₆ Câ€“H Bond Activation on TiO₂ via Combining First-Principles Ground-State and Excited-State Electronic Structure Calculations. Journal of Physical Chemistry Letters, 2022, 13, 6532-6540.	2.1	6
477	Structural and electrocatalytic properties of copper clusters: A study via deep learning and first principles. Journal of Chemical Physics, 2022, 157, .	1.2	6
478	Proposed mechanical method for switching the spin transport channel in two-dimensional magnetic metalâ€“magnetic semiconductor van der Waals contacts. Nanoscale Horizons, 2020, 5, 1496-1499.	4.1	5
479	Identifying the Molecular Orientation and Clusters in the Liquidâ€“Vapor Interface of 1-Propanol by Time-Delayed Mass Spectrometry. Journal of Physical Chemistry Letters, 2020, 11, 7510-7516.	2.1	5
480	The Moving-Grid Effect in the Harmonic Vibrational Frequency Calculations with Numeric Atom-Centered Orbitals. Journal of Physical Chemistry A, 2020, 124, 2897-2906.	1.1	5
481	CrSbS₃ monolayer: a potential phase transition ferromagnetic semiconductor. Nanoscale, 2021, 13, 14067-14072.	2.8	5
482	Topological phase transition driven by a spatially periodic potential. Physical Review B, 2014, 90, .	1.1	4
483	Spin Selection Rule in Single-Site Catalysis of Molecular Oxygen Adsorption on Transition-Metal Phthalocyanines. Journal of Physical Chemistry C, 2019, 123, 28158-28167.	1.5	4
484	Ion-molecule reactions catalyzed by a single gold atom. Chemical Science, 2020, 11, 8502-8505.	3.7	4
485	Hybrid MPI and OpenMP parallel implementation of large-scale linear-response time-dependent density functional theory with plane-wave basis set. Electronic Structure, 2021, 3, 024004.	1.0	4
486	An efficient implementation of spinâ€“orbit coupling within the framework of semiempirical orthogonalization-corrected methods for ultrafast intersystem crossing dynamics. Physical Chemistry Chemical Physics, 2021, 23, 22313-22323.	1.3	4

#	Article	IF	Citations
487	Implementation of Laplace Transformed MP2 for Periodic Systems With Numerical Atomic Orbitals. Frontiers in Chemistry, 2020, 8, 589992.	1.8	4
488	High-Throughput Computational Screening for Bipolar Magnetic Semiconductors. Research, 2022, 2022, 9857631.	2.8	4
489	Electronic, Optical, and Mechanical Properties of Diamond Nanowires Encapsulated in Carbon Nanotubes: A First-Principles View. Journal of Physical Chemistry C, 2017, 121, 3661-3672.	1.5	3
490	Transport properties of a three-shell icosahedral matryoshka cluster: a first-principles study. RSC Advances, 2017, 7, 12704-12710.	1.7	3
491	Spatial and thickness dependence of coupling interaction of surface states and influence on transport and optical properties of few-layer Bi2Se3. Journal of Physics Condensed Matter, 2018, 30, 065503.	0.7	3
492	Obtaining Intrinsically Occupied Free-Space Superatom States in an Encapsulated Ca2N Nanotube. ACS Omega, 2018, 3, 11966-11971.	1.6	3
493	Competitive Transient Electrostatic Adsorption for In Situ Regeneration of Poisoned Catalyst. ChemCatChem, 2019, 11, 1179-1184.	1.8	3
494	Oscillation of Work Function during Reducible Metal Oxide Catalysis and Correlation with the Activity Property. ChemCatChem, 2020, 12, 85-89.	1.8	3
495	Two-dimensional Ca4N2 as a one-dimensional electride [Ca4N2]2+Â·2eâˆ' with ultrahigh conductance. Nanoscale, 2020, 12, 5578-5586.	2.8	3
496	Capturing the Electronâ€"Phonon Renormalization in Molecules from First-Principles. Journal of Physical Chemistry A, 2021, 125, 2682-2689.	1.1	3
497	Exploring Accurate Potential Energy Surfaces via Integrating Variational Quantum Eigensolver with Machine Learning. Journal of Physical Chemistry Letters, 0, , 6420-6426.	2.1	3
498	A New Variational Method for the Coupling System of Polaron in a Quantum Well. Physica Status Solidi (B): Basic Research, 1999, 212, 271-279.	0.7	2
499	Magnetism of semiconductor-based magnetic tunnel junctions under electric field from first principles. Applied Physics Letters, 2009, 94, .	1.5	2
500	First Principles Study on FeAs Single Layers. Chinese Journal of Chemical Physics, 2009, 22, 139-142.	0.6	2
501	Chiral selective tunneling induced graphene nanoribbon switch. Frontiers of Physics in China, 2009, 4, 373-377.	1.0	2
502	High-Pressure Phase Favored by a Symmetry-Recognized Nanoconfinement Effect. Journal of Physical Chemistry Letters, 2012, 3, 2154-2158.	2.1	2
503	Spin-polarized transport properties of Mn@Au6 cluster. Chemical Physics Letters, 2013, 590, 111-115.	1.2	2
504	Ir Detectors: Ultrahigh Infrared Photoresponse from Core-Shell Single-Domain-VO2/V2O5Heterostructure in Nanobeam (Adv. Funct. Mater. 13/2014). Advanced Functional Materials, 2014, 24, 1820-1820.	7.8	2

#	Article	IF	Citations
505	The static parallel distribution algorithms for hybrid density-functional calculations in HONPAS package. International Journal of High Performance Computing Applications, 2020, 34, 159-168.	2.4	2
506	Parallel Implementation of Large-Scale Linear Scaling Density Functional Theory Calculations With Numerical Atomic Orbitals in HONPAS. Frontiers in Chemistry, 2020, 8, 589910.	1.8	2
507	In Situ Low-Temperature Growth and Superior Luminescent Property of Well-Aligned, High-Quality Cubic CsPbBr₃ Micrometer-Scale Single Crystal Arrays on Transparent Conductive Substrates. Journal of Physical Chemistry Letters, 2022, 13, 1114-1122.	2.1	2
508	Computational characterization of nanosystems. Chinese Journal of Chemical Physics, 2022, 35, 1-15.	0.6	2
509	Bipolar Magnetic Molecules for Spinâ€Polarized Electric Current in Molecular Junctions. Angewandte Chemie, 2022, 134, .	1.6	2
510	Fabrication of conjugated polymer arrays by spinodal dewetting. Polymer International, 2004, 53, 1968-1972.	1.6	1
511	POLARIZABILITY AND SHIELDING OF COAXIAL HYBRID DOUBLE-WALLED NANOTUBES: A FIRST-PRINCIPLES STUDY. Journal of Theoretical and Computational Chemistry, 2008, 07, 793-803.	1.8	1
512	Exploring at nanoscale from first principles. Frontiers of Physics in China, 2009, 4, 256-268.	1.0	1
513	Theoretical investigation on icosahedral C₆₀(FeCp)₁₂: A hybrid of C₆₀and ferrocene. International Journal of Quantum Chemistry, 2015, 115, 1621-1628.	1.0	1
514	In-gap localized states induced by adsorbates on silicene. Physical Review B, 2016, 93, .	1.1	1
515	Hidden Order and Haldane-Like Phase in Molecular Chains Assembled from Conformation-Switchable Molecules. ACS Nano, 2018, 12, 6515-6522.	7.3	1
516	Mixed magnetic edge states in graphene quantum dots. Multifunctional Materials, 2022, 5, 014001.	2.4	1
517	Controlling the Valenceâ€Electron Arrangement of Nickel Active Centers for Efficient Hydrogen Oxidation Electrocatalysis. Angewandte Chemie, 0, , .	1.6	1
518	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	0
519	First-principles Study of Adsorption and Dissociation of Methanol on the Pt(100) Surface. Chinese Journal of Chemical Physics, 2012, 25, 199-203.	0.6	0
520	RÃ¼cktitelbild: The Nanoparticle Size Effect in Graphene Cutting: A â€œPac-Manâ€• Mechanism (Angew. Chem.) Tj ETQq0 0 0 rgBT /Ove	1.6	0
521	Frontispiz: Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. Angewandte Chemie, 2018, 130, .	1.6	0
522	Frontispiece: Tuning Charge Transport in Aromatic-Ring Single-Molecule Junctions via Ionic-Liquid Gating. Angewandte Chemie - International Edition, 2018, 57, .	7.2	0

#	Article	IF	Citations
523	Preface: celebrating the 60th anniversary of the University of Science and Technology of China. Science China Chemistry, 2018, 61, 1043-1044.	4.2	0
524	Reaction on a Rink: Kondo-Enhanced Heterogeneous Single-Atom Catalysis. Journal of Physical Chemistry C, 0, , .	1.5	0
525	The Electronic State and Spatial Distribution of Excess Charge Created by Oxygen Vacancies on Titanium Dioxide Surfaces. Hyomen Kagaku, 2010, 31, 474-479.	0.0	0
526	The Journal of Physical Chemistry C Virtual Special Issue on â€œEnergy and Catalysis in Chinaâ€. Journal of Physical Chemistry C, 2022, 126, 2301-2306.	1.5	0