Yoshiyuki Kawazoe

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3530168/publications.pdf

Version: 2024-02-01

288	18,010	34016 52	14702 127
papers	citations	h-index	g-index

293	293	293	17849
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ordering and interatomic bonding in magnetostrictive Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e222" altimg="si1.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>0</mml:mn><mml:mo>.</mml:mo><mml:mn>85</mml:mn></mml:mrow></mml:msub></mml:math>Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e234" altimg="si2.svg"><mml:msub><mml:mrow />	1.4	3
2	First-principles identification of interface effect on Li storage capacity of C3N/graphene multilayer heterostructure. Journal of Colloid and Interface Science, 2022, 610, 80-88.	5.0	11
3	Intermolecular and Intramolecular Friedelâ€Crafts Acylation of Carboxylic Acids using Binary Ionic Liquids: An Experimental and Computational Study. ChemistrySelect, 2022, 7, .	0.7	5
4	Three-dimensional tetrahexcarbon: Stability and properties. Materials Today Physics, 2022, 23, 100628.	2.9	8
5	Effects of nanostructures on the hydrogen storage properties of MgH2 - A first principles study. Computational Condensed Matter, 2022, 30, e00643.	0.9	8
6	Mechanisms of Ionic Diffusion and Stability of the Na₄MnCr(PO₄)₃ Cathode. , 2022, 4, 860-867.		13
7	Exploration of glassy state in Prussian blue analogues. Nature Communications, 2022, 13, .	5.8	21
8	18 and 12 â€“ Member carbon rings (cyclo[n]carbons) â€“ A density functional study. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 263, 114895.	1.7	6
9	MXenes: Novel electrocatalysts for hydrogen production and nitrogen reduction. Catalysis Today, 2021, 370, 2-13.	2.2	22
10	Charge transfer driven interaction of CH4, CO2 and NH3 with TiS2 monolayer: Influence of vacancy defect. Catalysis Today, 2021, 370, 189-195.	2.2	5
11	Ab initio design of a new family of 2D materials: transition metal carbon nitrogen compounds (MCNs). Journal of Materials Chemistry C, 2021, 9, 4748-4756.	2.7	8
12	Creation of Mo/Tc@C60 and Au@C60 and molecular-dynamics simulations. RSC Advances, 2021, 11, 19666-19672.	1.7	3
13	Modulating Interfacial Charge Density of NiP₂â€“FeP₂ via Coupling with Metallic Cu for Accelerating Alkaline Hydrogen Evolution. ACS Energy Letters, 2021, 6, 354-363.	8.8	146
14	Effect of axial molecules and linker length on CO₂ adsorption and selectivity of CAU-8: a combined DFT and GCMC simulation study. RSC Advances, 2021, 11, 12460-12469.	1.7	0
15	First-principles study of a topological phase transition induced by image potential states in MXenes. Physical Review B, 2021, 103, .	1.1	6
16	Pentagonal transition-metal (group X) chalcogenide monolayers: Intrinsic semiconductors for photocatalysis. International Journal of Hydrogen Energy, 2021, 46, 9371-9379.	3.8	27
17	Uncovering the Role of Countercations in Ligand Exchange of WSe₂: Tuning the d-Band Center toward Improved Hydrogen Desorption. ACS Applied Materials & Interfaces, 2021, 13, 11403-11413.	4.0	15
18	A computational study on the complexation of bisbenzimidazolyl derivatives with cucurbituril and cyclohexylcucurbituril. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2021, 100, 217.	0.9	4

#	Article	IF	Citations
19	Improved Thermoelectric Performance of Cu₁₂Sb₄S₁₃ through Gd-Substitution Induced Enhancement of Electronic Density of States and Phonon Scattering. ACS Applied Materials & Interfaces, 2021, 13, 25092-25101.	4.0	18
20	Dissociation of hydrogen peroxide in water and methanol through a biased molecular dynamics investigation. Journal of Computational Chemistry, 2021, 42, 1344-1353.	1.5	6
21	Nitrogen doping in non-magnetic yttrium oxide: Induction of room temperature ferromagnetism from first principles simulations. Journal of Magnetism and Magnetic Materials, 2021, 528, 167840.	1.0	5
22	CNSi/MXene/CNSi: Unique Structure with Specific Electronic Properties for Nanodevices. Small, 2021, 17, 2101482.	5.2	2
23	Activityâ€“Selectivity Enhancement and Catalytic Trend of CO₂ Electroreduction on Metallic Dimers Supported by N-Doped Graphene: A Computational Study. Journal of Physical Chemistry C, 2021, 125, 13176-13184.	1.5	12
24	A theoretical investigation of quantum spin Hall state in ordered Mâ€²2Mâ€³2C3 MXenes (Mâ€² = V, Nb, Ta and Mâ€³) Tj ETQq0 0 0 rg	0.7	3
25	Atomistic origin of compositional pulling effect in wurtzite (B, Al, In)xGa1âˆ’xN: A first-principles study. Journal of Applied Physics, 2021, 130, 035704.	1.1	7
26	A theoretical investigation of topological phase modulation in carbide MXenes: Role of image potential states. Carbon, 2021, 181, 370-378.	5.4	6
27	Intermolecular interactions in microhydrated ribonucleoside and deoxyribonucleoside: A computational study. Computational and Theoretical Chemistry, 2021, 1204, 113422.	1.1	4
28	Hex-C558: A new porous metallic carbon allotrope for lithium-ion battery anode. Carbon, 2021, 183, 652-659.	5.4	10
29	A record high average ZT over a wide temperature range in a Single-layer Sb2Si2Te6. Applied Surface Science, 2021, 567, 150873.	3.1	3
30	Design of 2D materials â€“ MSi₂C_xN_{4âˆ’x} (M = Cr, Mo, and W;) Tj ETQq0 0 0 rgBT /Overlock 10	2.8	10
31	Boron-Functionalized Organic Framework as a High-Performance Metal-Free Catalyst for N₂ Fixation. Journal of Physical Chemistry Letters, 2021, 12, 12142-12149.	2.1	9
32	Transformation of hydrogen bond network during CO2 clathrate hydrate dissociation. Applied Surface Science, 2020, 499, 143644.	3.1	10
33	Low thermal conductivity of peanut-shaped carbon nanotube and its insensitive response to uniaxial strain. Nanotechnology, 2020, 31, 115701.	1.3	4
34	Boosting Electrocatalytic HER Activity of 3D Interconnected CoSP via Metal Doping: Active and Stable Electrocatalysts for pH-Universal Hydrogen Generation. Chemistry of Materials, 2020, 32, 9591-9601.	3.2	39
35	Potential of porous nodal-line semi-metallic carbon for sodium-ion battery anode. Journal of Power Sources, 2020, 478, 228746.	4.0	14
36	The electronic structures and magnetic properties of mixed-valence Fe-based metalâ€“organic VNU-15 frameworks: a theoretical study from linear response DFT+U calculations. RSC Advances, 2020, 10, 34690-34701.	1.7	1

#	Article	IF	Citations
37	Magnetic and electronic properties of 2D TiX3 (X = F, Cl, Br and I). Physical Chemistry Chemical Physics, 2020, 22, 17632-17638.	1.3	12
38	Tuning the electronic and magnetic properties of pentagraphene through the C1 vacancy. 2D Materials, 2020, 7, 045024.	2.0	6
39	A stable metallic 3D porous BPC₂ as a universal anode material for Li, Na, and K ion batteries with high performance. Journal of Materials Chemistry A, 2020, 8, 25824-25830.	5.2	18
40	Reaction probability and kinetics of water splitting on the penta-NiAs₂ monolayer from an ab initio molecular dynamics investigation. Physical Chemistry Chemical Physics, 2020, 22, 18149-18154.	1.3	2
41	Role of Methane as a Second Guest Component in Thermodynamic Stability and Isomer Selectivity of Butane Clathrate Hydrates. Journal of Physical Chemistry C, 2020, 124, 18474-18481.	1.5	17
42	Induced Magnetism of the MoS₂ Monolayer during the Transition Metal (Fe/Ni) Bombardment Process: A Nonadiabatic Ab Initio Collision Dynamics Investigation. ACS Omega, 2020, 5, 16139-16148.	1.6	0
43	Lattice Dynamics Study of the Thermal Expansion of C₃H₈-, CH₄-, CF₄-, CO₂-, Xe-, and N₂-Hydrates. Energy & Fuels, 2020, 34, 12771-12778.	2.5	10
44	Design of novel pentagonal 2D transitional-metal sulphide monolayers for hydrogen evolution reaction. International Journal of Hydrogen Energy, 2020, 45, 16201-16209.	3.8	32
45	Exotic properties of materials and the necessity to invoke the dimension of angle (?) and the orbital degrees of freedom of s electrons. International Journal of Computational Materials Science and Engineering, 2020, 09, 2050003.	0.5	2
46	Modulation of nearly free electron states in hydroxyl-functionalized MXenes: a first-principles study. Journal of Materials Chemistry C, 2020, 8, 5211-5221.	2.7	21
47	Triphenylene and tetracene based porous sheet: Stability and electronic properties. Computational Materials Science, 2020, 176, 109529.	1.4	4
48	Graphdiyneâ€Based Monolayers as Promising Anchoring Materials for Lithiumâ€“Sulfur Batteries: A Theoretical Study. Advanced Theory and Simulations, 2020, 3, 1900236.	1.3	21
49	Microwave-assisted synthesis of nano Hf- and Zr-based metal-organic frameworks for enhancement of curcumin adsorption. Microporous and Mesoporous Materials, 2020, 298, 110064.	2.2	74
50	Design of tetracene-based metallic 2D carbon materials for Na- and K-Ion batteries. Applied Surface Science, 2020, 521, 146456.	3.1	40
51	The nano-structural inhomogeneity of dynamic hydrogen bond network of TIP4P/2005 water. Scientific Reports, 2020, 10, 7323.	1.6	13
52	Penta-BCN: A New Ternary Pentagonal Monolayer with Intrinsic Piezoelectricity. Journal of Physical Chemistry Letters, 2020, 11, 3501-3506.	2.1	80
53	Non-regular hexagonal 2D carbon, an allotrope of graphene: a first-principles computational study. Journal of Molecular Modeling, 2020, 26, 150.	0.8	3
54	A proton transfer mechanism along the PO₄ anion chain in the [Zn(HPO₄)(H₂PO₄)]^{2â^'} coordination polymer. Physical Chemistry Chemical Physics, 2019, 21, 18605-18611.	1.3	3

#	Article	IF	Citations
55	Tuning the Properties of Tetraceneâ€Based Nanoribbons by Fluorination and Nâ€Doping. ChemPhysChem, 2019, 20, 2799-2805.	1.0	10
56	Synergistic Effects of Nitrogen Doping on MXene for Enhancement of Hydrogen Evolution Reaction. ACS Sustainable Chemistry and Engineering, 2019, 7, 16879-16888.	3.2	130
57	A superhard orthorhombic carbon with all six-membered-ring in sp3 bonding networks. Physics Letters, Section A: General, Atomic and Solid State Physics, 2019, 383, 2809-2812.	0.9	19
58	Nanoparticle Linkerâ€Controlled Molecular Wire Devices Based on Double Molecular Monolayers. Small, 2019, 15, 1901183.	5.2	9
59	N-doped peanut-shaped carbon nanotubes for efficient CO2 electrocatalytic reduction. Carbon, 2019, 152, 241-246.	5.4	29
60	Oriented Attachment Revisited: Does a Chemical Reaction Occur?. Matter, 2019, 1, 690-704.	5.0	27
61	Zr and Hf-metal-organic frameworks: Efficient and recyclable heterogeneous catalysts for the synthesis of 2-arylbenzoxazole via ring open pathway acylation reaction. Journal of Catalysis, 2019, 374, 110-117.	3.1	27
62	Adsorption and Diffusion of H Atoms on Î²-PtO₂ Surface: The Role of Nuclear Quantum Effects. Journal of Physical Chemistry C, 2019, 123, 13804-13811.	1.5	9
63	Phase diagram and composition of water based crystalline phases in hydrogen â€“ Water binary system. Solid State Communications, 2019, 294, 6-10.	0.9	10
64	Applications of aesthetic pentagon-shaped stereo tiling employing pentagraphene carbonâ€”star walls and embossment design. AIP Advances, 2019, 9, 035001.	0.6	1
65	Magnetism in two-dimensional materials beyond graphene. Materials Today, 2019, 27, 107-122.	8.3	127
66	A theoretical exploration of the intermolecular interactions between resveratrol and water: a DFT and AIM analysis. Journal of Molecular Modeling, 2019, 25, 56.	0.8	14
67	Design of pentagonal NbX monolayers for electronics and electrocatalysis. Applied Surface Science, 2019, 479, 595-600.	3.1	14
68	Interfacial properties of penta-graphene-metal contacts. Journal of Applied Physics, 2019, 125, .	1.1	11
69	Electron delocalization in single-layer phthalocyanine-based covalent organic frameworks: a first principle study. RSC Advances, 2019, 9, 29440-29447.	1.7	11
70	Adsorption of water on fluorinated graphene. Journal of Physics and Chemistry of Solids, 2019, 124, 54-59.	1.9	16
71	Thermal transport properties of penta-graphene with grain boundaries. Carbon, 2019, 145, 445-451.	5.4	20
72	Tunable Band Gaps of In_xGa_{1â€“x}N Alloys: From Bulk to Two-Dimensional Limit. Journal of Physical Chemistry C, 2018, 122, 6930-6942.	1.5	35

#	Article	IF	Citations
73	Ozone storage capacity in clathrate hydrates formed by O₃+ O₂+ N₂+ CO₂gas mixtures. Physical Chemistry Chemical Physics, 2018, 20, 12637-12641.	1.3	37
74	Ab Initio Methods. , 2018, , 7-197.		2
75	A metallic peanut-shaped carbon nanotube and its potential for CO2 capture. Carbon, 2018, 132, 249-256.	5.4	13
76	Penetrating probability and cross section of the Li+â€“C60 encapsulation process through an ab initio molecular dynamics investigation. Physical Chemistry Chemical Physics, 2018, 20, 7007-7013.	1.3	1
77	Anionâ€“Cation Double Substitution in Transition Metal Dichalcogenide to Accelerate Water Dissociation Kinetic for Electrocatalysis. Advanced Energy Materials, 2018, 8, 1702139.	10.2	70
78	New carbon allotropes in sp + sp³ bonding networks consisting of C₈ cubes. Physical Chemistry Chemical Physics, 2018, 20, 7962-7967.	1.3	33
79	Bipolar Magnetic Materials Based on 2D Ni[TCNE] Metalâ€“Organic Coordination Networks. Advanced Electronic Materials, 2018, 4, 1700323.	2.6	17
80	Topological Nodal-Net Semimetal in a Graphene Network Structure. Physical Review Letters, 2018, 120, 026402.	2.9	93
81	Extensive first-principles molecular dynamics study on Li encapsulation into C₆₀ and its experimental confirmation. Nanoscale, 2018, 10, 1825-1836.	2.8	3
82	Theoretical insights into the minority carrier lifetime of doped Siâ€”A computational study. Journal of Applied Physics, 2018, 123, 161420.	1.1	2
83	Unravelling the nature of binding of cubane and substituted cubanes within cucurbiturils: A DFT and NCI study. Journal of Molecular Liquids, 2018, 260, 18-29.	2.3	52
84	Exploring new two-dimensional monolayers: pentagonal transition metal borides/carbides (penta-TMB/Cs). Journal of Materials Chemistry A, 2018, 6, 10226-10232.	5.2	77
85	First principle study on the Si effect in the Fe-based soft magnetic nano-crystalline alloys. Journal of Alloys and Compounds, 2018, 730, 196-200.	2.8	11
86	Monoclinic C16: sp-sp hybridized nodal-line semimetal protected by PT-symmetry. Carbon, 2018, 127, 527-532.	5.4	32
87	Density functional theory study on the dihydrogen bond cooperativity in the growth behavior of dimethyl sulfoxide clusters. Journal of Molecular Liquids, 2018, 249, 454-462.	2.3	30
88	Ab initio molecular dynamics simulations of nano-crystallization of Fe-based amorphous alloys with early transition metals. Chinese Physics B, 2018, 27, 116401.	0.7	2
89	Monitoring Mechanical, Electronic, and Catalytic Trends in a Titanium Metal Organic Framework Under the Influence of Guest-Molecule Encapsulation Using Density Functional Theory. Scientific Reports, 2018, 8, 16651.	1.6	12
90	Influence of N2 on Formation Conditions and Guest Distribution of Mixed CO2 + CH4 Gas Hydrates. Molecules, 2018, 23, 3336.	1.7	34

#	Article	IF	Citations
91	Clathrate hydrates for energy storage and transportation. Journal of Physics: Conference Series, 2018, 1128, 012031.	0.3	14
92	From Reticular Chemistry Design to Density Functional Theory Modeling for New Zeolitic Imidazolate Framework Topologies: Mechanical Stability, Electronic Structure, and CO₂ Selectivity. Journal of Physical Chemistry C, 2018, 122, 23543-23553.	1.5	4
93	Adsorption and diffusion of F 2 molecules on pristine graphene. Chinese Physics B, 2018, 27, 106801.	0.7	6
94	Reticular control of interpenetration in a complex metalâ€“organic framework. Materials Chemistry Frontiers, 2018, 2, 2063-2069.	3.2	15
95	Topological nodal line semimetal in an orthorhombic graphene network structure. Physical Review B, 2018, 97, .	1.1	29
96	Room-temperature <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>d</mml:mi><mml:mn>0</mml:mn></mml:msup></mml:m ferromagnetism in carbon-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Y</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> for s	1.1	22
97	Two-dimensional pentagonal CrX (X = S, Se or Te) monolayers: antiferromagnetic semiconductors for spintronics and photocatalysts. Physical Chemistry Chemical Physics, 2018, 20, 18348-18354.	1.3	26
98	A new 3D Dirac nodal-line semi-metallic graphene monolith for lithium ion battery anode materials. Journal of Materials Chemistry A, 2018, 6, 13816-13824.	5.2	44
99	Tuning the electronic and magnetic properties of graphene/h-BN hetero nanoribbon: A first-principles investigation. AIP Advances, 2018, 8, .	0.6	7
100	Prediction of new ground-state crystal structure of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">T</mml:mi><mml:msub><mml:mi mathvariant="normal">a</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review Materials, 2018, 2, .	0.9	19
101	Ab initio direct dynamics of transition metal atom/dimers bombardments onto graphene: Evolution of magnetic alignment. Carbon, 2017, 115, 791-802.	5.4	2
102	Improvement of dopant distribution in radial direction of single crystals grown by micro-pulling-down method. Journal of Crystal Growth, 2017, 474, 178-182.	0.7	7
103	Bodyâ€Centered Tetragonal C₁₆: A Novel Topological Nodeâ€Line Semimetallic Carbon Composed of Tetrarings. Small, 2017, 13, 1602894.	5.2	65
104	Asian consortium on computational materials science theme meeting on â€œfirst principles analysis & experiment: Role in energy researchâ€•22â€“24 september 2016, SRM University, Kattankulathur, Chennai, India (ACCMS-TM 2016). Applied Surface Science, 2017, 418, 1.	3.1	1
105	Gamma (Î³)-ray irradiated multi-walled carbon nanotubes (MWCNTs) for hydrogen storage. Applied Surface Science, 2017, 418, 49-55.	3.1	41
106	High pressure band gap modification of LiCaAlF6. Applied Physics Letters, 2017, 110, .	1.5	15
107	Effects of dopant distribution improvement on optical and scintillation properties for Ce-doped garnet-type single crystals. Journal of Materials Science: Materials in Electronics, 2017, 28, 7151-7156.	1.1	8
108	Effect of Elasticity of the MoS₂ Surface on Li Atom Bouncing and Migration: Mechanism from Ab Initio Molecular Dynamic Investigations. Journal of Physical Chemistry C, 2017, 121, 1329-1338.	1.5	3

#	Article	IF	Citations
109	First-principles modeling of metal (ii) ferrocyanide: electronic property, magnetism, bulk moduli, and the role of Câ€‰â€‰â‰¡â€‰â€‰N^{â^'}defect. Journal Physics D: Applied Physics, 2017, 50, 035004.	1.3	3
110	Intermolecular interaction in nucleobases and dimethyl sulfoxide/water molecules: A DFT, NBO, AIM and NCI analysis. Journal of Molecular Graphics and Modelling, 2017, 78, 48-60.	1.3	73
111	Exceptional Thermoelectric Properties of Layered GeAs₂. Chemistry of Materials, 2017, 29, 9300-9307.	3.2	80
112	Atomistic observation of the collision and migration of Li on MoSe₂ and WS₂ surfaces through ab initio molecular dynamics. Physical Chemistry Chemical Physics, 2017, 19, 27332-27342.	1.3	3
113	Fabrication of poly(ethylene glycol) hydrogels containing vertically and horizontally aligned graphene using dielectrophoresis: An experimental and modeling study. Carbon, 2017, 123, 460-470.	5.4	24
114	Polarons in endohedral Li+@C60- dimers and in 1D and 2D crystals. Solid State Communications, 2017, 265, 1-5.	0.9	0
115	Quantum scar and breakdown of universality in graphene: A theoretical insight. International Journal of Modern Physics B, 2017, 31, 1750257.	1.0	0
116	Weak interlayer dependence of lattice thermal conductivity on stacking thickness of penta-graphene. Applied Physics Letters, 2017, 111, .	1.5	20
117	Theoretical prediction of two-dimensional functionalized MXene nitrides as topological insulators. Physical Review B, 2017, 96, .	1.1	83
118	Interaction of Pyrene Ligands with Neat and Defective Two Dimensional ZnO: A First Principles Study. MRS Advances, 2017, 2, 2799-2805.	0.5	0
119	First-principles calculations of electronic and optical properties of LiCaAlF 6 and LiSrAlF 6 crystals as VUV to UV solid-state laser materials. Optical Materials, 2017, 65, 15-20.	1.7	19
120	Adjusting band gap and charge transfer of organometallic complex adsorbed on MoS₂monolayer using vertical electric-field: a first-principles investigation. Journal of Physics Condensed Matter, 2017, 29, 015003.	0.7	2
121	The prospect of sensitizing organic dyes attached to the MoS2 surface: Physical insights from density functional theory investigations. Chemical Physics Letters, 2017, 667, 290-295.	1.2	6
122	Origin of magnetism â€" 90 Years of misunderstanding. , 2017, , .		0
123	Three-Dimensional Carbon Allotropes Comprising Phenyl Rings and Acetylenic Chains in sp+sp2 Hybrid Networks. Scientific Reports, 2016, 6, 24665.	1.6	29
124	Hidden electronic rule in the â€œcluster-plus-glue-atomâ€•model. Scientific Reports, 2016, 6, 33672.	1.6	10
125	Investigation on the crystallization mechanism difference between FINEMETÂ® and NANOMETÂ® type Fe-based soft magnetic amorphous alloys. Journal of Applied Physics, 2016, 120, 145102.	1.1	22
126	First-principles modeling of 3d-transition-metal-atom adsorption on silicene: a linear-response DFTâ€‰â€‰+â€‰â€‰Uapproach. Journal of Physics Condensed Matter, 2016, 28, 135301.	0.7	13

#	Article	IF	Citations
127	Conceptual design of tetraazaporphyrin- and subtetraazaporphyrin-based functional nanocarbon materials: electronic structures, topologies, optical properties, and methane storage capacities. Physical Chemistry Chemical Physics, 2016, 18, 13503-13518.	1.3	3
128	Lattice thermal conductivity of penta-graphene. Carbon, 2016, 105, 424-429.	5.4	120
129	Intrinsic quantum spin Hall and anomalous Hall effects in h-Sb/Bi epitaxial growth on a ferromagnetic MnO₂thin film. Nanoscale, 2016, 8, 11202-11209.	2.8	16
130	Global minimum of two-dimensional FeB₆and an oxidization induced negative Poisson's ratio: a new stable allotrope. Journal of Materials Chemistry C, 2016, 4, 9613-9621.	2.7	29
131	Multiple unpinned Dirac points in group-Va single-layers with phosphorene structure. Npj Computational Materials, 2016, 2, .	3.5	57
132	Ferromagnetic and Half-Metallic FeC₂ Monolayer Containing C₂ Dimers. ACS Applied Materials & Interfaces, 2016, 8, 26207-26212.	4.0	58
133	Effect of multiple defects and substituted impurities on the band structure of graphene: a DFT study. Journal of Materials Science: Materials in Electronics, 2016, 27, 12669-12679.	1.1	13
134	Body-Centered Orthorhombic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow><mml:mrow><mml:mn>16</mml:mn></mml:mrow></mml:msub></mml:mrow></mm A Novel Topological Node-Line Semimetal. Physical Review Letters, 2016, 116, 195501.	2.9	170
135	Dirac cone move and bandgap on/off switching of graphene superlattice. Scientific Reports, 2016, 6, 18869.	1.6	24
136	DFT Study of Carbon Crystals from Nested K4 Lattice to BCâ€8 Structure. Journal of the Chinese Chemical Society, 2016, 63, 526-532.	0.8	1
137	Electrochemical Potential Derived from Atomic Cluster Structures. Journal of Physical Chemistry Letters, 2016, 7, 567-571.	2.1	9
138	Three Dimensional Metallic Carbon from Distorting sp³-Bond. Crystal Growth and Design, 2016, 16, 1360-1365.	1.4	39
139	Novel three dimensional topological nodal line semimetallic carbon. Carbon, 2016, 98, 468-473.	5.4	36
140	Interaction of VOCs with pyrene tetratopic ligands layered on ZnO nanorods under visible light. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 324, 62-69.	2.0	17
141	CO Oxidation Prefers the Eleyâ€“Rideal or Langmuirâ€“Hinshelwood Pathway: Monolayer vs Thin Film of SiC. ACS Applied Materials & Interfaces, 2016, 8, 5290-5299.	4.0	44
142	Simulation on Thermocapillary-Driven Drop Coalescence by Hybrid Lattice Boltzmann Method. Microgravity Science and Technology, 2016, 28, 67-77.	0.7	16
143	Ab Initio Investigation of Oâ€“H Dissociation from the Alâ€“OH₂ Complex Using Molecular Dynamics and Neural Network Fitting. Journal of Physical Chemistry A, 2016, 120, 346-355.	1.1	10
144	Hydrogen hydrates: Equation of state and self-preservation effect. Fluid Phase Equilibria, 2016, 413, 220-228.	1.4	39

#	Article	IF	Citations
145	The selectivity and activity of catalyst for CO hydrogenation to methanol and hydrocarbon: A comparative study on Cu, Co and Ni surfaces. Surface Science, 2016, 645, 30-40.	0.8	15
146	Effect of surface doping on the band structure of graphene: a DFT study. Journal of Materials Science: Materials in Electronics, 2016, 27, 2728-2740.	1.1	16
147	Numerical study on the radial dopant distribution in micro-pulling-down crystal growth. Journal of Crystal Growth, 2016, 434, 110-115.	0.7	7
148	Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers. Physical Chemistry Chemical Physics, 2016, 18, 8777-8784.	1.3	273
149	Topological node-line semimetal in three-dimensional graphene networks. Physical Review B, 2015, 92, .	1.1	619
150	Large-gap two-dimensional topological insulator in oxygen functionalized MXene. Physical Review B, 2015, 92, .	1.1	229
151	A New Silicon Phase with Direct Band Gap and Novel Optoelectronic Properties. Scientific Reports, 2015, 5, 14342.	1.6	74
152	Activation of CO and CO2 on homonuclear boron bonds of fullerene-like BN cages: first principles study. Scientific Reports, 2015, 5, 17460.	1.6	36
153	Computational study on the interactions of mustard gas with cucurbituril macrocycles. International Journal of Quantum Chemistry, 2015, 115, 1515-1525.	1.0	23
154	Giant magnetocrystalline anisotropy of 5d transition metal-based phthalocyanine sheet. Physical Chemistry Chemical Physics, 2015, 17, 17182-17189.	1.3	19
155	Effects of metalloids in Fe-rich soft magnetic amorphous alloys on magnetization. , 2015, , .		1
156	Comparison of the electronic band structures of LiCaAlF₆and LiSrAlF₆ultraviolet laser host media from ab initio calculations. Japanese Journal of Applied Physics, 2015, 54, 122602.	0.8	13
157	Electrically Tunable In-Plane Anisotropic Magnetoresistance in Topological Insulator BiSbTeSe₂ Nanodevices. Nano Letters, 2015, 15, 2061-2066.	4.5	56
158	TOMBO: All-electron mixed-basis approach to condensed matter physics. Computer Physics Communications, 2015, 189, 20-30.	3.0	28
159	Porphyrin-based porous sheet: Optoelectronic properties and hydrogen storage. International Journal of Hydrogen Energy, 2015, 40, 3689-3696.	3.8	22
160	Native point defects in few-layer phosphorene. Physical Review B, 2015, 91, .	1.1	104
161	Facile and green production of aqueous graphene dispersions for biomedical applications. Nanoscale, 2015, 7, 6436-6443.	2.8	114
162	Penta-graphene: A new carbon allotrope. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2372-2377.	3.3	1,114

#	Article	IF	Citations
163	Phase stability and transition of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>BaSi</mml:mtext><mml:mn>2</mml:mn></mml:msub disilicides and digermanides. Physical Review B, 2015, 91, .		
164	Sources ofn-type conductivity in GaInO₃. Journal Physics D: Applied Physics, 2015, 48, 015101.	1.3	13
165	First-principle simulation on the crystallization tendency and enhanced magnetization of Fe₇₆B₁₉P₅ amorphous alloy. Materials Research Express, 2015, 2, 016506.	0.8	8
166	Selective gas adsorption in microporous metalâ€“organic frameworks incorporating urotropine basic sites: an experimental and theoretical study. Chemical Communications, 2015, 51, 13918-13921.	2.2	29
167	Magnetic Influence of Alloying Elements in Fe-Rich Amorphous Alloys Studied by <italic>Ab Initio</italic> Molecular Dynamics Simulations. IEEE Transactions on Magnetics, 2015, 51, 1-4.	1.2	1
168	First principles modeling of Ag adsorption on the LaMnO3 (001) surfaces. Solid State Ionics, 2015, 273, 46-50.	1.3	1
169	An alternative second order scheme for curved boundary condition in lattice Boltzmann method. Computers and Fluids, 2015, 114, 193-202.	1.3	14
170	Cluster characteristics and physical properties of binary Alâ€“Zr intermetallic compounds from first principles studies. Computational Materials Science, 2015, 103, 170-178.	1.4	30
171	Functionalized single-walled carbon nanotube (5, 0) as a carrier for isoniazid â€" A tuberculosis drug. International Journal of Computational Materials Science and Engineering, 2015, 04, 1550014.	0.5	3
172	Solvation Mechanism of Task-Specific Ionic Liquids in Water: A Combined Investigation Using Classical Molecular Dynamics and Density Functional Theory. Journal of Physical Chemistry B, 2015, 119, 12894-12904.	1.2	16
173	Atomic packing and diffusion in Fe85Si2B9P4 amorphous alloy analyzed by ab initio molecular dynamics simulation. Journal of Applied Physics, 2015, 117, .	1.1	7
174	Theoretical Modeling of Oxygen and Water Adsorptionon Indium Oxide (111) Surface. ACS Symposium Series, 2015, , 137-149.	0.5	4
175	New Phosphorene Allotropes Containing Ridges with 2- and 4-Coordination. Journal of Physical Chemistry C, 2015, 119, 24674-24680.	1.5	37
176	Band Gap on/off Switching of Silicene Superlattice. Journal of Physical Chemistry C, 2015, 119, 20747-20754.	1.5	21
177	Mechanical and thermal properties of Î³-Mg2SiO4 under high temperature and high pressure conditions such as in mantle: A first principles study. Journal of Chemical Physics, 2015, 143, 104503.	1.2	14
178	Role of Interlayer Coupling on the Evolution of Band Edges in Few-Layer Phosphorene. Journal of Physical Chemistry Letters, 2015, 6, 4876-4883.	2.1	38
179	Self-assembly of metal atoms (Na, K, Ca) on graphene. Nanoscale, 2015, 7, 2352-2359.	2.8	10
180	First Principles Study on Structural Stability of Belite. ACI Materials Journal, 2015, 112, .	0.3	3

#	Article	IF	Citations
181	Effect of Nature of Dopants on Electronic and Optical Properties of Indium Tin Oxide. Advanced Science Letters, 2015, 21, 2697-2700.	0.2	0
182	Nano-crystallization and magnetic mechanisms of Fe85Si2B8P4Cu1 amorphous alloy by ab initio molecular dynamics simulation. Journal of Applied Physics, 2014, 115, .	1.1	17
183	Theoretical study of hydrogen storage in binary hydrogen-methane clathrate hydrates. Journal of Renewable and Sustainable Energy, 2014, 6, .	0.8	23
184	Lithium-doped triazine-based graphitic C3N4 sheet for hydrogen storage at ambient temperature. Computational Materials Science, 2014, 81, 275-279.	1.4	75
185	Structural and Magnetic Study of <inline-formula> <tex-math notation="TeX">${m Fe}_{76}{m Si}_{9}{m B}_{10}{m P}_{5}$ </tex-math></inline-formula> Metallic Glass by First Principle Simulation. IEEE Transactions on Magnetics, 2014, 50, 1-4.	1.2	3
186	Theoretical investigation of structures, compositions, and phase transitions of neon hydrates based on ices Ih and II. Journal of Engineering Thermophysics, 2014, 23, 20-26.	0.6	5
187	Theoretical investigation of structures and compositions of double neon-methane clathrate hydrates, depending on gas phase composition and pressure. Journal of Engineering Thermophysics, 2014, 23, 9-19.	0.6	8
188	Degenerate Perturbation in Band-Gap Opening of Graphene Superlattice. Journal of Physical Chemistry C, 2014, 118, 8174-8180.	1.5	15
189	Hydrogen storage in TiO2 functionalized (10, 10) single walled carbon nanotube (SWCNT) â€“ First principles study. International Journal of Hydrogen Energy, 2014, 39, 4973-4980.	3.8	26
190	Structures and Phase Transition of a MoS₂ Monolayer. Journal of Physical Chemistry C, 2014, 118, 1515-1522.	1.5	432
191	Phase stability, elastic and electronic properties of Cuâ€“Zr binary system intermetallic compounds: A first-principles study. Journal of Alloys and Compounds, 2014, 588, 96-102.	2.8	64
192	Theoretical evaluation on solubility of synthesized task specific ionic liquids in water. Journal of Molecular Liquids, 2014, 200, 232-237.	2.3	8
193	An alternative lattice Boltzmann model for three-dimensional incompressible flow. Computers and Mathematics With Applications, 2014, 68, 1107-1122.	1.4	2
194	Tuning electronic and magnetic properties of silicene with magnetic superhalogens. Physical Chemistry Chemical Physics, 2014, 16, 22979-22986.	1.3	35
195	Electronic properties of silicene superlattices: roles of degenerate perturbation and inversion symmetry breaking. Journal of Materials Chemistry C, 2014, 2, 8773-8779.	2.7	13
196	An effective method of tuning conducting properties: First-principles studies on electronic structures of graphene nanomeshes. Carbon, 2014, 79, 646-653.	5.4	18
197	Exceptionally long-ranged lattice relaxation in oxygen-deficient Ta2O5. Solid State Communications, 2014, 195, 16-20.	0.9	10
198	Nanostructures of C₆₀â€”Metalâ€”Graphene (Metal = Ti, Cr, Mn, Fe, or Ni): A Spin-Polarized Density Functional Theory Study. Journal of Physical Chemistry C, 2014, 118, 21057-21065.	1.5	14

#	Article	IF	Citations
199	Stability and properties of 2D porous nanosheets based on tetraoxa[8]circulene analogues. Nanoscale, 2014, 6, 14962-14970.	2.8	27
200	First-principles studies on structural, mechanical, thermodynamic and electronic properties of Niâ€“Zr intermetallic compounds. Intermetallics, 2014, 54, 110-119.	1.8	64
201	Stability and Composition of Helium Hydrates Based on Ices I_h and II at Low Temperatures. Journal of Physical Chemistry C, 2014, 118, 2587-2593.	1.5	27
202	Negatively curved cubic carbon crystals with octahedral symmetry. Carbon, 2014, 76, 266-274.	5.4	48
203	Engineering of Band Gap in Metalâ€“Organic Frameworks by Functionalizing Organic Linker: A Systematic Density Functional Theory Investigation. Journal of Physical Chemistry C, 2014, 118, 4567-4577.	1.5	97
204	Determining characteristic principal clusters in the â€œcluster-plus-glue-atomâ€•model. Acta Materialia, 2014, 75, 113-121.	3.8	34
205	A New Carbon Allotrope with Six-Fold Helical Chains in all-sp2 Bonding Networks. Scientific Reports, 2014, 4, 4339.	1.6	77
206	Effect of a nickel dimer on the dissociation dynamics of a hydrogen molecule. RSC Advances, 2013, 3, 12307.	1.7	3
207	Roles of oxygen vacancy on ferromagnetism in Ni doped In2O3: A hybrid functional study. Journal of Magnetism and Magnetic Materials, 2013, 348, 55-60.	1.0	5
208	Three-Dimensional Metallic Boron Nitride. Journal of the American Chemical Society, 2013, 135, 18216-18221.	6.6	145
209	The Intrinsic Ferromagnetism in a MnO₂ Monolayer. Journal of Physical Chemistry Letters, 2013, 4, 3382-3386.	2.1	171
210	Novel Electronic and Magnetic Properties of Twoâ€Đimensional Transition Metal Carbides and Nitrides. Advanced Functional Materials, 2013, 23, 2185-2192.	7.8	1,418
211	Temperature and pressure dependent geometry optimization and elastic constant calculations for arbitrary symmetry crystals: Applications to MgSiO3 perovskites. Journal of Applied Physics, 2013, 113, .	1.1	23
212	New Carbon Allotropes with Helical Chains of Complementary Chirality Connected by Ethene-type Ï€-Conjugation. Scientific Reports, 2013, 3, 3077.	1.6	52
213	Kinetic Origin of Divergent Decompression Pathways in Silicon and Germanium. Physical Review Letters, 2013, 110, 165503.	2.9	44
214	First principles study of hydrogen storage in SWCNT functionalized with MgH[sub 2]. , 2013, , .		1
215	First-principles study of exohedral and substitutional chemical functionalization of graphene. , 2012, , .		3
216	Tuning Electronic Structure of Graphene: A First-Principles Study. IEEE Nanotechnology Magazine, 2012, 11, 534-541.	1.1	37

#	Article	IF	Citations
217	Strain-Induced Spin Crossover in Phthalocyanine-Based Organometallic Sheets. Journal of Physical Chemistry Letters, 2012, 3, 3109-3114.	2.1	54
218	Phase conversion from graphite toward a simple monoclinic sp3-carbon allotrope. Journal of Chemical Physics, 2012, 137, 024502.	1.2	38
219	Simulation of ripples in single layer graphene sheets and study of their vibrational and elastic properties. Computational Materials Science, 2012, 51, 96-102.	1.4	18
220	Calcium-decorated graphene for hydrogen storage: A van der Waals density functional study. Computational Materials Science, 2012, 55, 180-185.	1.4	33
221	Theoretical investigation of ozone hydrate formation conditions. Journal of Structural Chemistry, 2012, 53, 627-633.	0.3	7
222	Theoretical modelling of the phase diagrams of clathrate hydrates for hydrogen storage applications. Molecular Simulation, 2012, 38, 773-780.	0.9	20
223	Band gap engineering of silicene zigzag nanoribbons with perpendicular electric fields: a theoretical study. Journal of Physics Condensed Matter, 2012, 24, 455302.	0.7	33
224	Theoretical Prediction of the Complexation Behaviors of Antitumor Platinum Drugs with Cucurbiturils. Journal of Physical Chemistry B, 2012, 116, 14029-14039.	1.2	42
225	Orthorhombic carbon allotrope of compressed graphite:Ab initiocalculations. Physical Review B, 2012, 85, .	1.1	80
226	New cubic carbon phase via graphitic sheet rumpling. Physical Review B, 2012, 85, .	1.1	30
227	Temperature dependent elastic constants for crystals with arbitrary symmetry: Combined first principles and continuum elasticity theory. Journal of Applied Physics, 2012, 111, .	1.1	46
228	Cucurbit[7]uril encapsulated cisplatin overcomes cisplatin resistance via a pharmacokinetic effect. Metallomics, 2012, 4, 561.	1.0	90
229	First-principles study of intrinsic defect properties in hexagonal BN bilayer and monolayer. Solid State Communications, 2012, 152, 816-820.	0.9	34
230	Noncovalent and covalent functionalization of a (5, 0) single-walled carbon nanotube with alanine and alanine radicals. Journal of Molecular Modeling, 2012, 18, 771-781.	0.8	19
231	Mechanism for direct conversion of graphite to diamond. Physical Review B, 2011, 84, .	1.1	34
232	Interaction of valine and valine radicals with single-walled carbon nanotube (5,0). Chemical Physics Letters, 2011, 511, 299-303.	1.2	11
233	Low-Temperature Phase Transformation from Graphite to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:math>Orthorhombic Carbon. Physical Review Letters, 2011, 106, 075501.	2.9	259
234	Thermodynamic stability of C3H8 hydrate of cubic structure IV using lattice dynamics. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2011, 69, 281-286.	1.6	1

#	Article	IF	Citations
235	Carbon-doped K4 nitrogen: A novel high energy density material. Chemical Physics Letters, 2011, 506, 175-178.	1.2	6
236	Pressure-dependent mechanical stability of simple cubic carbon. Physica B: Condensed Matter, 2011, 406, 2654-2657.	1.3	6
237	First principles investigation on carbon nanostructures functionalized with borane: An analysis on their hydrogen storage capacity. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1528-1534.	1.3	9
238	Theoretical insights into the formation, structure, and electronic properties of anticancer oxaliplatin drug and cucurbit[n]urils nÂ=Â5 to 8. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2010, 66, 213-218.	1.6	54
239	Modular, Homochiral, Porous Coordination Polymers: Rational Design, Enantioselective Guest Exchange Sorption and Ab Initio Calculations of Hostâ€“Guest Interactions. Chemistry - A European Journal, 2010, 16, 10348-10356.	1.7	67
240	The role of Li and Ni metals in the adsorbate complex and their effect on the hydrogen storage capacity of single walled carbon nanotubes coated with metal hydrides, LiH and NiH2. International Journal of Hydrogen Energy, 2010, 35, 2368-2376.	3.8	38
241	Theoretical investigation on the alkali-metal doped BN fullerene as a material for hydrogen storage. Chemical Physics, 2010, 377, 54-59.	0.9	39
242	Phase stability of carbon clathrates at high pressure. Journal of Applied Physics, 2010, 107, .	1.1	31
243	Thermodynamic phase behavior of binary clathrate hydrates: Computational prediction. Computational Materials Science, 2010, 49, S187-S193.	1.4	8
244	Accurate description of phase diagram of clathrate hydrates at the molecular level. Journal of Chemical Physics, 2009, 131, 244510.	1.2	44
245	Hydrogen storage capacity of C60(OM)12 (M=Li and Na) clusters. Journal of Chemical Physics, 2009, 131, 214505.	1.2	41
246	Theoretical Study of Hydrogen Storage in Ca-Coated Fullerenes. Journal of Chemical Theory and Computation, 2009, 5, 374-379.	2.3	130
247	Theoretical study of phase transitions in Kr and Ar clathrate hydrates from structure II to structure I under pressure. Journal of Chemical Physics, 2009, 131, 114507.	1.2	43
248	Ferromagnetism in Semihydrogenated Graphene Sheet. Nano Letters, 2009, 9, 3867-3870.	4.5	771
249	New Metallic Carbon Crystal. Physical Review Letters, 2009, 102, 055703.	2.9	119
250	A theoretical study on the interaction of aromatic amino acids with graphene and single walled carbon nanotube. Journal of Chemical Physics, 2009, 130, 124911.	1.2	251
251	Electron-capture decay rate of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mmultiscripts><mml:mtext>B</mml:mtext><mml:mprescripts /><mml:none /><mml:mn>7</mml:mn></mml:mmultiscripts><mml:mtext>e</mml:mtext><mml:mo>@</mml:mo><mml:msub><mml:mtext>C</mml:mtext> first-principles calculations based on density functional theory. Physical Review B, 2008, 78, .	1.1	16
252	Physical and Chemical Properties of Gas Hydrates: Theoretical Aspects of Energy Storage Application. Materials Transactions, 2007, 48, 704-710.	0.4	59

#	Article	IF	Citations
253	First-principles study of the structural, electronic, and elastic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>R</mml:mi><mml:msub><mml:mi mathvariant="normal">Rh</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi		

#	Article	IF	Citations
271	All-Electron Mixed-Basis Calculation of Structurally Optimized Titanium Nitride Clusters. Materials Transactions, 2002, 43, 482-484.	0.4	5
272	Formation of N-doped C₆₀ Studied by <I>Ab Initio</I> Molecular Dynamics Simulations. Materials Transactions, 2001, 42, 2189-2193.	0.4	9
273	All-Electron Mixed-Basis Calculation to Optimize Structures of Vanadium Clusters. Materials Transactions, 2001, 42, 432-434.	0.4	4
274	Three-dimensional oscillatory thermocapillary convection in liquid bridge under microgravity. International Journal of Heat and Mass Transfer, 2001, 44, 3765-3774.	2.5	25
275	Ab initioGWquasiparticle energies of small sodium clusters by an all-electron mixed-basis approach. Physical Review B, 2001, 63, .	1.1	46
276	Absolute total energy of small copper clusters in an all-electron mixed-basis approach with the generalized-gradient approximation. Journal of Materials Research, 1999, 14, 980-983.	1.2	2
277	Ab initiostudy of phonons in hexagonal GaN. Physical Review B, 1999, 60, 15511-15514.	1.1	43
278	Direct numerical simulation of oscillatory Marangoni convection in cylindrical liquid bridges. Journal of Crystal Growth, 1999, 204, 395-404.	0.7	32
279	In-situ infrared spectroscopy of a photoirradiated potassium-doped C60 film. Chemical Physics Letters, 1999, 315, 19-24.	1.2	22
280	Ab Initio study of dopant insertion into carbon nanotubes. Journal of Chemical Physics, 1999, 111, 2164-2168.	1.2	44
281	Formation of As- and Ge-doped heterofullerenes. Physical Review B, 1999, 60, 1531-1534.	1.1	38
282	All-Electron Mixed-Basis Calculation with Conjugated Gradient Method to Optimize Structure of Copper Clusters. Materials Transactions, JIM, 1999, 40, 1205-1208.	0.9	3
283	Insertion of Xe and Kr Atoms into C60 and C70 Fullerenes and the Formation of Dimers. Physical Review Letters, 1998, 81, 967-970.	2.9	102
284	Vibrational modes and IR analysis of neutral photopolymerizedC60dimers. Physical Review B, 1998, 57, 223-229.	1.1	62
285	First-Principles Determination of the Soft Mode in CubicZrO2. Physical Review Letters, 1997, 78, 4063-4066.	2.9	2,341
286	Ab InitioMolecular Dynamics Simulations for Collision betweenC60â^'and Alkali-Metal Ions: A Possibility of Li@C60. Physical Review Letters, 1996, 76, 3590-3593.	2.9	85
287	Insertion of Be Atoms inC60Fullerene Cages:Be@C60. Physical Review Letters, 1996, 77, 3522-3524.	2.9	118
288	Intramolecular structures ofC60molecules adsorbed on the Cu(111)-(1Ã—1) surface. Physical Review Letters, 1993, 71, 2959-2962.	2.9	241