Yoshiyuki Kawazoe

List of Publications by Year
in descending order

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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	First-Principles Determination of the Soft Mode in CubicZrO2. Physical Review Letters, 1997, 78, 4063-4066.	2.9	2,341
2	Novel Electronic and Magnetic Properties of Twoâ€Dimensional Transition Metal Carbides and Nitrides. Advanced Functional Materials, 2013, 23, 2185-2192.	7.8	1,418
3	Highly controlled acetylene accommodation in a metalâ€“organic microporous material. Nature, 2005, 436, 238-241.	13.7	1,386
4	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
5	Ferromagnetism in Semihydrogenated Graphene Sheet. Nano Letters, 2009, 9, 3867-3870.	4.5	771
6	Clustering of Ti on a C60Surface and Its Effect on Hydrogen Storage. Journal of the American Chemical Society, 2005, 127, 14582-14583.	6.6	675
7	Topological node-line semimetal in three-dimensional graphene networks. Physical Review B, 2015, 92, .	1.1	619
8	Ultra-stable nanoparticles of CdSe revealed from mass spectrometry. Nature Materials, 2004, 3, 99-102.	13.3	469
9	Structures and Phase Transition of a MoS₂ Monolayer. Journal of Physical Chemistry C, 2014, 118, 1515-1522.	1.5	432
10	Exfoliating biocompatible ferromagnetic Cr-trihalide monolayers. Physical Chemistry Chemical Physics, 2016, 18, 8777-8784.	1.3	273
11	Low-Temperature Phase Transformation from Graphite to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>s</mml:mi><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
12	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
13	Intramolecular structures ofC60molecules adsorbed on the Cu(111)-(1Ã—1) surface. Physical Review Letters, 1993, 71, 2959-2962.	2.9	241
14	Large-gap two-dimensional topological insulator in oxygen functionalized MXene. Physical Review B, 2015, 92, .	1.1	229
15	The Intrinsic Ferromagnetism in a MnO₂ Monolayer. Journal of Physical Chemistry Letters, 2013, 4, 3382-3386.	2.1	171
16	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></mml:math>A Novel Topological Node-Line Semimetal. Physical Review Letters, 2016, 116, 195501.	2.9	170
17	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
18	Three-Dimensional Metallic Boron Nitride. Journal of the American Chemical Society, 2013, 135, 18216-18221.	6.6	145

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19	Theoretical Study of Hydrogen Storage in Ca-Coated Fullerenes. Journal of Chemical Theory and Computation, 2009, 5, 374-379.	2.3	130
20	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
21	Magnetism in two-dimensional materials beyond graphene. Materials Today, 2019, 27, 107-122.	8.3	127
22	Lattice thermal conductivity of penta-graphene. Carbon, 2016, 105, 424-429.	5.4	120
23	New Metallic Carbon Crystal. Physical Review Letters, 2009, 102, 055703.	2.9	119
24	Insertion of Be Atoms inC60Fullerene Cages:Be@C60. Physical Review Letters, 1996, 77, 3522-3524.	2.9	118
25	Facile and green production of aqueous graphene dispersions for biomedical applications. Nanoscale, 2015, 7, 6436-6443.	2.8	114
26	Native point defects in few-layer phosphorene. Physical Review B, 2015, 91, .	1.1	104
27	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
28	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
29	Topological Nodal-Net Semimetal in a Graphene Network Structure. Physical Review Letters, 2018, 120, 026402.	2.9	93
30	Cucurbit[7]uril encapsulated cisplatin overcomes cisplatin resistance via a pharmacokinetic effect. Metallomics, 2012, 4, 561.	1.0	90
31	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
32	Theoretical prediction of two-dimensional functionalized MXene nitrides as topological insulators. Physical Review B, 2017, 96, .	1.1	83
33	Orthorhombic carbon allotrope of compressed graphite:Ab initiocalculations. Physical Review B, 2012, 85, .	1.1	80
34	Exceptional Thermoelectric Properties of Layered GeAs₂. Chemistry of Materials, 2017, 29, 9300-9307.	3.2	80
35	Penta-BCN: A New Ternary Pentagonal Monolayer with Intrinsic Piezoelectricity. Journal of Physical Chemistry Letters, 2020, 11, 3501-3506.	2.1	80
36	A New Carbon Allotrope with Six-Fold Helical Chains in all-sp2 Bonding Networks. Scientific Reports, 2014, 4, 4339.	1.6	77

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37	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
38	Lithium-doped triazine-based graphitic C3N4 sheet for hydrogen storage at ambient temperature. Computational Materials Science, 2014, 81, 275-279.	1.4	75
39	A New Silicon Phase with Direct Band Gap and Novel Optoelectronic Properties. Scientific Reports, 2015, 5, 14342.	1.6	74
40	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
41	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
42	Anionâ€“Cation Double Substitution in Transition Metal Dichalcogenide to Accelerate Water Dissociation Kinetic for Electrocatalysis. Advanced Energy Materials, 2018, 8, 1702139.	10.2	70
43	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
44	Bodyâ€€centered Tetragonal C₁₆: A Novel Topological Nodeâ€Ł ine Semimetallic Carbon Composed of Tetrarings. Small, 2017, 13, 1602894.	5.2	65
45	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
46	First-principles studies on structural, mechanical, thermodynamic and electronic properties of Niâ€“Zr intermetallic compounds. Intermetallics, 2014, 54, 110-119.	1.8	64
47	Vibrational modes and IR analysis of neutral photopolymerizedC60dimers. Physical Review B, 1998, 57, 223-229.	1.1	62
48	Physical and Chemical Properties of Gas Hydrates: Theoretical Aspects of Energy Storage Application. Materials Transactions, 2007, 48, 704-710.	0.4	59
49	Ferromagnetic and Half-Metallic FeC₂ Monolayer Containing C₂ Dimers. ACS Applied Materials & Interfaces, 2016, 8, 26207-26212.	4.0	58
50	Multiple unpinned Dirac points in group-Va single-layers with phosphorene structure. Npj Computational Materials, 2016, 2, .	3.5	57
51	Electrically Tunable In-Plane Anisotropic Magnetoresistance in Topological Insulator BiSbTeSe₂ Nanodevices. Nano Letters, 2015, 15, 2061-2066.	4.5	56
52	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
53	Strain-Induced Spin Crossover in Phthalocyanine-Based Organometallic Sheets. Journal of Physical Chemistry Letters, 2012, 3, 3109-3114.	2.1	54
54	New Carbon Allotropes with Helical Chains of Complementary Chirality Connected by Ethene-type Ï€-Conjugation. Scientific Reports, 2013, 3, 3077.	1.6	52

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55	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
56	Negatively curved cubic carbon crystals with octahedral symmetry. Carbon, 2014, 76, 266-274.	5.4	48
57	Ab initioGWquasiparticle energies of small sodium clusters by an all-electron mixed-basis approach. Physical Review B, 2001, 63, .	1.1	46
58	Ab initio GWquasiparticle calculation of small alkali-metal clusters. Physical Review B, 2002, 65, .	1.1	46
59	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
60	Proposed design principle of fluoride-based materials for deep ultraviolet light emitting devices. Optical Materials, 2007, 30, 15-17.	1.7	45
61	Ab Initio study of dopant insertion into carbon nanotubes. Journal of Chemical Physics, 1999, 111, 2164-2168.	1.2	44
62	Accurate description of phase diagram of clathrate hydrates at the molecular level. Journal of Chemical Physics, 2009, 131, 244510.	1.2	44
63	Kinetic Origin of Divergent Decompression Pathways in Silicon and Germanium. Physical Review Letters, 2013, 110, 165503.	2.9	44
64	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
65	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
66	Ab initiostudy of phonons in hexagonal GaN. Physical Review B, 1999, 60, 15511-15514.	1.1	43
67	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
68	Ab Initio Study of Hydrogen Storage in Hydrogen Hydrate Clathrates. Materials Transactions, 2004, 45, 1452-1454.	0.4	42
69	Theoretical Prediction of the Complexation Behaviors of Antitumor Platinum Drugs with Cucurbiturils. Journal of Physical Chemistry B, 2012, 116, 14029-14039.	1.2	42
70	Hydrogen storage capacity of C60(OM)12 (M=Li and Na) clusters. Journal of Chemical Physics, 2009, 131, 214505.	1.2	41
71	Gamma (Î³)-ray irradiated multi-walled carbon nanotubes (MWCNTs) for hydrogen storage. Applied Surface Science, 2017, 418, 49-55.	3.1	41
72	Design of tetracene-based metallic 2D carbon materials for Na- and K-Ion batteries. Applied Surface Science, 2020, 521, 146456.	3.1	40

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73	Dynamics and equation of state of hydrogen clathrate hydrate as a function of cage occupation. Computational Materials Science, 2006, 36, 229-233.	1.4	39
74	Theoretical investigation on the alkali-metal doped BN fullerene as a material for hydrogen storage. Chemical Physics, 2010, 377, 54-59.	0.9	39
75	Three Dimensional Metallic Carbon from Distorting sp³-Bond. Crystal Growth and Design, 2016, 16, 1360-1365.	1.4	39
76	Hydrogen hydrates: Equation of state and self-preservation effect. Fluid Phase Equilibria, 2016, 413, 220-228.	1.4	39
77	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
78	Formation of As- and Ge-doped heterofullerenes. Physical Review B, 1999, 60, 1531-1534.	1.1	38
79	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
80	Phase conversion from graphite toward a simple monoclinic sp3-carbon allotrope. Journal of Chemical Physics, 2012, 137, 024502.	1.2	38
81	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
82	Tuning Electronic Structure of Graphene: A First-Principles Study. IEEE Nanotechnology Magazine, 2012, 11, 534-541.	1.1	37
83	New Phosphorene Allotropes Containing Ridges with 2- and 4-Coordination. Journal of Physical Chemistry C, 2015, 119, 24674-24680.	1.5	37
84	Ozone storage capacity in clathrate hydrates formed by O₃+ O₂+ N₂+ CO₂gas mixtures. Physical Chemistry Chemical Physics, 2018, 20, 12637-12641.	1.3	37
85	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
86	Novel three dimensional topological nodal line semimetallic carbon. Carbon, 2016, 98, 468-473.	5.4	36
87	Tuning electronic and magnetic properties of silicene with magnetic superhalogens. Physical Chemistry Chemical Physics, 2014, 16, 22979-22986.	1.3	35
88	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
89	Mechanism for direct conversion of graphite to diamond. Physical Review B, 2011, 84, .	1.1	34
90	First-principles study of intrinsic defect properties in hexagonal BN bilayer and monolayer. Solid State Communications, 2012, 152, 816-820.	0.9	34

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91	Determining characteristic principal clusters in the â€œcluster-plus-glue-atomâ€•model. Acta Materialia, 2014, 75, 113-121.	3.8	34
92	Influence of N2 on Formation Conditions and Guest Distribution of Mixed CO2 + CH4 Gas Hydrates. Molecules, 2018, 23, 3336.	1.7	34
93	Calcium-decorated graphene for hydrogen storage: A van der Waals density functional study. Computational Materials Science, 2012, 55, 180-185.	1.4	33
94	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
95	New carbon allotropes in sp + sp³ bonding networks consisting of C₈ cubes. Physical Chemistry Chemical Physics, 2018, 20, 7962-7967.	1.3	33
96	Direct numerical simulation of oscillatory Marangoni convection in cylindrical liquid bridges. Journal of Crystal Growth, 1999, 204, 395-404.	0.7	32
97	Monoclinic C16: sp-sp hybridized nodal-line semimetal protected by PT-symmetry. Carbon, 2018, 127, 527-532.	5.4	32
98	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
99	Phase stability of carbon clathrates at high pressure. Journal of Applied Physics, 2010, 107, .	1.1	31
100	First-principles calculations of hyperfine parameters with the all-electron mixed-basis method. Physical Review B, 2006, 73, .	1.1	30
101	New cubic carbon phase via graphitic sheet rumpling. Physical Review B, 2012, 85, .	1.1	30
102	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
103	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
104	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
105	Three-Dimensional Carbon Allotropes Comprising Phenyl Rings and Acetylenic Chains in sp+sp2 Hybrid Networks. Scientific Reports, 2016, 6, 24665.	1.6	29
106	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
107	Topological nodal line semimetal in an orthorhombic graphene network structure. Physical Review B, 2018, 97, .	1.1	29
108	N-doped peanut-shaped carbon nanotubes for efficient CO2 electrocatalytic reduction. Carbon, 2019, 152, 241-246.	5.4	29

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109	TOMBO: All-electron mixed-basis approach to condensed matter physics. Computer Physics Communications, 2015, 189, 20-30.	3.0	28
110	Stability and properties of 2D porous nanosheets based on tetraoxa[8]circulene analogues. Nanoscale, 2014, 6, 14962-14970.	2.8	27
111	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
112	Oriented Attachment Revisited: Does a Chemical Reaction Occur?. Matter, 2019, 1, 690-704.	5.0	27
113	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
114	Pentagonal transition-metal (group X) chalcogenide monolayers: Intrinsic semiconductors for photocatalysis. International Journal of Hydrogen Energy, 2021, 46, 9371-9379.	3.8	27
115	Breakdown of time-reversal symmetry of photoemission and its inverse in small silicon clusters. Physical Review B, 2003, 68, .	1.1	26
116	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
117	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
118	Three-dimensional oscillatory thermocapillary convection in liquid bridge under microgravity. International Journal of Heat and Mass Transfer, 2001, 44, 3765-3774.	2.5	25
119	Dirac cone move and bandgap on/off switching of graphene superlattice. Scientific Reports, 2016, 6, 18869.	1.6	24
120	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
121	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:mi		

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127	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
128	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
129	MXenes: Novel electrocatalysts for hydrogen production and nitrogen reduction. Catalysis Today, 2021, 370, 2-13.	2.2	22
130	Band Gap on/off Switching of Silicene Superlattice. Journal of Physical Chemistry C, 2015, 119, 20747-20754.	1.5	21
131	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
132	Graphdiyneâ€Based Monolayers as Promising Anchoring Materials for Lithiumâ€“Sulfur Batteries: A Theoretical Study. Advanced Theory and Simulations, 2020, 3, 1900236.	1.3	21
133	Exploration of glassy state in Prussian blue analogues. Nature Communications, 2022, 13, .	5.8	21
134	Theoretical modelling of the phase diagrams of clathrate hydrates for hydrogen storage applications. Molecular Simulation, 2012, 38, 773-780.	0.9	20
135	Weak interlayer dependence of lattice thermal conductivity on stacking thickness of penta-graphene. Applied Physics Letters, 2017, 111, .	1.5	20
136	Thermal transport properties of penta-graphene with grain boundaries. Carbon, 2019, 145, 445-451.	5.4	20
137	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
138	Giant magnetocrystalline anisotropy of 5d transition metal-based phthalocyanine sheet. Physical Chemistry Chemical Physics, 2015, 17, 17182-17189.	1.3	19
139	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
140	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
141	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
142	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
143	An effective method of tuning conducting properties: First-principles studies on electronic structures of graphene nanomeshes. Carbon, 2014, 79, 646-653.	5.4	18
144	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

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145	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
146	First-principles study of Laâ€“B36N36 cage. Physica B: Condensed Matter, 2003, 339, 105-109.	1.3	17
147	Stoichiometric and ultra-stable nanoparticles of II-VI compound semiconductors. European Physical Journal D, 2005, 34, 39-41.	0.6	17
148	Nano-crystallization and magnetic mechanisms of Fe85Si2B8P4Cu1 amorphous alloy by ab initio molecular dynamics simulation. Journal of Applied Physics, 2014, 115, .	1.1	17
149	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
150	Bipolar Magnetic Materials Based on 2D Ni[TCNE] Metalâ€“Organic Coordination Networks. Advanced Electronic Materials, 2018, 4, 1700323.	2.6	17
151	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
152	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: first-principles calculations based on density functional theory. Physical Review B, 2008, 78, .	1.1	16
153	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
154	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
155	Simulation on Thermocapillary-Driven Drop Coalescence by Hybrid Lattice Boltzmann Method. Microgravity Science and Technology, 2016, 28, 67-77.	0.7	16
156	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
157	Adsorption of water on fluorinated graphene. Journal of Physics and Chemistry of Solids, 2019, 124, 54-59.	1.9	16
158	Degenerate Perturbation in Band-Gap Opening of Graphene Superlattice. Journal of Physical Chemistry C, 2014, 118, 8174-8180.	1.5	15
159	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
160	High pressure band gap modification of LiCaAlF6. Applied Physics Letters, 2017, 110, .	1.5	15
161	Reticular control of interpenetration in a complex metalâ€“organic framework. Materials Chemistry Frontiers, 2018, 2, 2063-2069.	3.2	15
162	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

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163	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
164	An alternative second order scheme for curved boundary condition in lattice Boltzmann method. Computers and Fluids, 2015, 114, 193-202.	1.3	14
165	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
166	Clathrate hydrates for energy storage and transportation. Journal of Physics: Conference Series, 2018, 1128, 012031.	0.3	14
167	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
168	Design of pentagonal NbX monolayers for electronics and electrocatalysis. Applied Surface Science, 2019, 479, 595-600.	3.1	14
169	Potential of porous nodal-line semi-metallic carbon for sodium-ion battery anode. Journal of Power Sources, 2020, 478, 228746.	4.0	14
170	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
171	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
172	Sources ofn-type conductivity in GaInO₃. Journal Physics D: Applied Physics, 2015, 48, 015101.	1.3	13
173	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
174	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
175	A metallic peanut-shaped carbon nanotube and its potential for CO2 capture. Carbon, 2018, 132, 249-256.	5.4	13
176	The nano-structural inhomogeneity of dynamic hydrogen bond network of TIP4P/2005 water. Scientific Reports, 2020, 10, 7323.	1.6	13
177	Mechanisms of Ionic Diffusion and Stability of the Na₄MnCr(PO₄)₃ Cathode. , 2022, 4, 860-867.		13
178	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
179	Magnetic and electronic properties of 2D TiX3 (X = F, Cl, Br and I). Physical Chemistry Chemical Physics, 2020, 22, 17632-17638.	1.3	12
180	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

#	Article	IF	Citations
181	Interaction of valine and valine radicals with single-walled carbon nanotube (5,0). Chemical Physics Letters, 2011, 511, 299-303.	1.2	11
182	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
183	Interfacial properties of penta-graphene-metal contacts. Journal of Applied Physics, 2019, 125, .	1.1	11
184	Electron delocalization in single-layer phthalocyanine-based covalent organic frameworks: a first principle study. RSC Advances, 2019, 9, 29440-29447.	1.7	11
185	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
186	Polaron in a one-dimensionalC60crystal. Physical Review B, 2003, 67, .	1.1	10
187	Exceptionally long-ranged lattice relaxation in oxygen-deficient Ta2O5. Solid State Communications, 2014, 195, 16-20.	0.9	10
188	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, .	1.1	10
189	Self-assembly of metal atoms (Na, K, Ca) on graphene. Nanoscale, 2015, 7, 2352-2359.	2.8	10
190	Hidden electronic rule in the â€œcluster-plus-glue-atomâ€•model. Scientific Reports, 2016, 6, 33672.	1.6	10
191	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
192	Tuning the Properties of Tetraceneâ€Based Nanoribbons by Fluorination and Nâ€Doping. ChemPhysChem, 2019, 20, 2799-2805.	1.0	10
193	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
194	Transformation of hydrogen bond network during CO2 clathrate hydrate dissociation. Applied Surface Science, 2020, 499, 143644.	3.1	10
195	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
196	Hex-C558: A new porous metallic carbon allotrope for lithium-ion battery anode. Carbon, 2021, 183, 652-659.	5.4	10
197	Design of 2D materials â€“ MSi₂C_xN_{4â^'x} (M = Cr, Mo, and W;) Tj ETQq1 1 0.784314 rgBT /Ov	2.8	10
198	Formation of N-doped C₆₀ Studied by <I>Ab Initio</I> Molecular Dynamics Simulations. Materials Transactions, 2001, 42, 2189-2193.	0.4	9

#	Article	IF	Citations
199	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
200	Electrochemical Potential Derived from Atomic Cluster Structures. Journal of Physical Chemistry Letters, 2016, 7, 567-571.	2.1	9
201	Nanoparticle Linkerâ€Controlled Molecular Wire Devices Based on Double Molecular Monolayers. Small, 2019, 15, 1901183.	5.2	9
202	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
203	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
204	Se atom incorporation in fullerenes by using nuclear recoil andab initiomolecular dynamics simulation. Physical Review B, 2002, 65, .	1.1	8
205	Thermodynamic phase behavior of binary clathrate hydrates: Computational prediction. Computational Materials Science, 2010, 49, S187-S193.	1.4	8
206	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
207	Theoretical evaluation on solubility of synthesized task specific ionic liquids in water. Journal of Molecular Liquids, 2014, 200, 232-237.	2.3	8
208	First-principle simulation on the crystallization tendency and enhanced magnetization of Fe₇₆B₁₉P₅ amorphous alloy. Materials Research Express, 2015, 2, 016506.	0.8	8
209	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
210	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
211	Three-dimensional tetrahexcarbon: Stability and properties. Materials Today Physics, 2022, 23, 100628.	2.9	8
212	Effects of nanostructures on the hydrogen storage properties of MgH2 - A first principles study. Computational Condensed Matter, 2022, 30, e00643.	0.9	8
213	First-principles calculations of optical absorption spectra of atoms in the vacuum and crystals. Computational Materials Science, 2006, 36, 125-129.	1.4	7
214	Theoretical investigation of ozone hydrate formation conditions. Journal of Structural Chemistry, 2012, 53, 627-633.	0.3	7
215	Atomic packing and diffusion in Fe85Si2B9P4 amorphous alloy analyzed by ab initio molecular dynamics simulation. Journal of Applied Physics, 2015, 117, .	1.1	7
216	Numerical study on the radial dopant distribution in micro-pulling-down crystal growth. Journal of Crystal Growth, 2016, 434, 110-115.	0.7	7

#	Article	IF	Citations
217	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
218	Tuning the electronic and magnetic properties of graphene/h-BN hetero nanoribbon: A first-principles investigation. AIP Advances, 2018, 8, .	0.6	7
219	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
220	Carbon-doped K4 nitrogen: A novel high energy density material. Chemical Physics Letters, 2011, 506, 175-178.	1.2	6
221	Pressure-dependent mechanical stability of simple cubic carbon. Physica B: Condensed Matter, 2011, 406, 2654-2657.	1.3	6
222	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
223	Adsorption and diffusion of F 2 molecules on pristine graphene. Chinese Physics B, 2018, 27, 106801.	0.7	6
224	Tuning the electronic and magnetic properties of pentagraphene through the C1 vacancy. 2D Materials, 2020, 7, 045024.	2.0	6
225	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
226	First-principles study of a topological phase transition induced by image potential states in MXenes. Physical Review B, 2021, 103, .	1.1	6
227	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
228	A theoretical investigation of topological phase modulation in carbide MXenes: Role of image potential states. Carbon, 2021, 181, 370-378.	5.4	6
229	All-Electron Mixed-Basis Calculation of Structurally Optimized Titanium Nitride Clusters. Materials Transactions, 2002, 43, 482-484.	0.4	5
230	Simulation of a chemical reaction, 2LiHâ†'Li2+H2, driven by doubly excitation. Science and Technology of Advanced Materials, 2004, 5, 609-611.	2.8	5
231	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
232	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
233	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
234	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

#	Article	IF	Citations
235	Intermolecular and Intramolecular Friedelâ€Crafts Acylation of Carboxylic Acids using Binary Ionic Liquids: An Experimental and Computational Study. ChemistrySelect, 2022, 7, .	0.7	5
236	All-Electron Mixed-Basis Calculation to Optimize Structures of Vanadium Clusters. Materials Transactions, 2001, 42, 432-434.	0.4	4
237	Double ionization energy spectra of small alkali-metal clusters. Science and Technology of Advanced Materials, 2004, 5, 663-665.	2.8	4
238	Theoretical Modeling of Oxygen and Water Adsorptionon Indium Oxide (111) Surface. ACS Symposium Series, 2015, , 137-149.	0.5	4
239	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
240	Low thermal conductivity of peanut-shaped carbon nanotube and its insensitive response to uniaxial strain. Nanotechnology, 2020, 31, 115701.	1.3	4
241	Triphenylene and tetracene based porous sheet: Stability and electronic properties. Computational Materials Science, 2020, 176, 109529.	1.4	4
242	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
243	Intermolecular interactions in microhydrated ribonucleoside and deoxyribonucleoside: A computational study. Computational and Theoretical Chemistry, 2021, 1204, 113422.	1.1	4
244	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
245	First-principles study of exohedral and substitutional chemical functionalization of graphene. , 2012, , .		3
246	Effect of a nickel dimer on the dissociation dynamics of a hydrogen molecule. RSC Advances, 2013, 3, 12307.	1.7	3
247	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
248	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
249	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
250	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
251	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
252	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

#	Article	IF	Citations
253	Extensive first-principles molecular dynamics study on Li encapsulation into C₆₀ and its experimental confirmation. Nanoscale, 2018, 10, 1825-1836.	2.8	3
254	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
255	Creation of Mo/Tc@C60 and Au@C60 and molecular-dynamics simulations. RSC Advances, 2021, 11, 19666-19672.	1.7	3
256	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
257	A record high average ZT over a wide temperature range in a Single-layer Sb2Si2Te6. Applied Surface Science, 2021, 567, 150873.	3.1	3
258	Non-regular hexagonal 2D carbon, an allotrope of graphene: a first-principles computational study. Journal of Molecular Modeling, 2020, 26, 150.	0.8	3
259	First Principles Study on Structural Stability of Belite. ACI Materials Journal, 2015, 112, .	0.3	3
260	Local 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<mm xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e234" altimg="si2.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>0</mml:mn><mml:mo>.</mml:mo><m	1.4	3
261	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
262	Theoretical study of polarons and self-trapped excited states in one-dimensional C60 crystal. Computational Materials Science, 2006, 36, 17-25.	1.4	2
263	An alternative lattice Boltzmann model for three-dimensional incompressible flow. Computers and Mathematics With Applications, 2014, 68, 1107-1122.	1.4	2
264	Ab initio direct dynamics of transition metal atom/dimers bombardments onto graphene: Evolution of magnetic alignment. Carbon, 2017, 115, 791-802.	5.4	2
265	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
266	Ab Initio Methods. , 2018, , 7-197.		2
267	Theoretical insights into the minority carrier lifetime of doped Siâ€”A computational study. Journal of Applied Physics, 2018, 123, 161420.	1.1	2
268	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
269	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
270	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

#	Article	IF	Citations
271	CNSi/MXene/CNSi: Unique Structure with Specific Electronic Properties for Nanodevices. Small, 2021, 17, 2101482.	5.2	2
272	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
273	First principles study of hydrogen storage in SWCNT functionalized with MgH[sub 2]. , 2013, , .		1
274	Effects of metalloids in Fe-rich soft magnetic amorphous alloys on magnetization. , 2015, , .		1
275	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
276	First principles modeling of Ag adsorption on the LaMnO3 (001) surfaces. Solid State Ionics, 2015, 273, 46-50.	1.3	1
277	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
278	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
279	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
280	Applications of aesthetic pentagon-shaped stereo tiling employing pentagraphene carbonâ€”star walls and embossment design. AIP Advances, 2019, 9, 035001.	0.6	1
281	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
282	Polarons in endohedral Li+@C60- dimers and in 1D and 2D crystals. Solid State Communications, 2017, 265, 1-5.	0.9	0
283	Quantum scar and breakdown of universality in graphene: A theoretical insight. International Journal of Modern Physics B, 2017, 31, 1750257.	1.0	0
284	Interaction of Pyrene Ligands with Neat and Defective Two Dimensional ZnO: A First Principles Study. MRS Advances, 2017, 2, 2799-2805.	0.5	0
285	Origin of magnetism â€” 90 Years of misunderstanding. , 2017, , .		0
286	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
287	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
288	Effect of Nature of Dopants on Electronic and Optical Properties of Indium Tin Oxide. Advanced Science Letters, 2015, 21, 2697-2700.	0.2	0