Cai-Zhuang Wang

List of Publications by Year
in descending order

285 papers	9,953 citations	38720 50 h-index	46771 89 g-index
299 all docs	299 docs citations	299 times ranked	9421 citing authors

#	Article	IF	Citations
1	Structures of medium-sized silicon clusters. Nature, 1998, 392, 582-585.	13.7	622
2	Diffusion, Coalescence, and Reconstruction of Vacancy Defects in Graphene Layers. Physical Review Letters, 2005, 95, 205501.	2.9	472
3	Melting line of aluminum from simulations of coexisting phases. Physical Review B, 1994, 49, 3109-3115.	1.1	438
4	Structure, dynamics, and electronic properties of diamondlike amorphous carbon. Physical Review Letters, 1993, 71, 1184-1187.	2.9	255
5	Phase Modulation of (1Tâ€2H)â€MoSe2/TiCâ€C Shell/Core Arrays via Nitrogen Doping for Highly Efficient Hydrogen Evolution Reaction. Advanced Materials, 2018, 30, e1802223.	11.1	244
6	Firstâ€principles study, fabrication, and characterization of (Hf_{0.2}Zr_{0.2}Ta_{0.2}Nb_{0.2}Ti_{0.2})C highâ€entropy ceramic. Journal of the American Ceramic Society, 2019, 102, 4344-4352.	1.9	217
7	On-the-fly machine-learning for high-throughput experiments: search for rare-earth-free permanent magnets. Scientific Reports, 2014, 4, 6367.	1.6	212
8	Tight-binding molecular-dynamics study of phonon anharmonic effects in silicon and diamond. Physical Review B, 1990, 42, 11276-11283.	1.1	172
9	Bonding and charge transfer by metal adatom adsorption on graphene. Physical Review B, 2011, 83, .	1.1	167
10	Molecule intrinsic minimal basis sets. I. Exact resolution ofab initiooptimized molecular orbitals in terms of deformed atomic minimal-basis orbitals. Journal of Chemical Physics, 2004, 120, 2629-2637.	1.2	155
11	The geometry of small fullerene cages: C20 to C70. Journal of Chemical Physics, 1992, 97, 5007-5011.	1.2	145
12	Tight-binding molecular-dynamics study of amorphous carbon. Physical Review Letters, 1993, 70, 611-614.	2.9	145
13	Metals on graphene: correlation between adatom adsorption behavior and growth morphology. Physical Chemistry Chemical Physics, 2012, 14, 9157.	1.3	145
14	Metals on Graphene: Interactions, Growth Morphology, and Thermal Stability. Crystals, 2013, 3, 79-111.	1.0	135
15	Broadband optical absorption by tunable Mie resonances in silicon nanocone arrays. Scientific Reports, 2015, 5, 7810.	1.6	126
16	Structures of Germanium Clusters: Where the Growth Patterns of Silicon and Germanium Clusters Diverge. Physical Review Letters, 1999, 83, 2167-2170.	2.9	123
17	Growth morphology and properties of metals on graphene. Progress in Surface Science, 2015, 90, 397-443.	3.8	123
18	Atomistic cluster alignment method for local order mining in liquids and glasses. Physical Review B, 2010, 82, .	1.1	120

#	Article	IF	Citations
19	An adaptive genetic algorithm for crystal structure prediction. Journal of Physics Condensed Matter, 2014, 26, 035402.	0.7	120
20	Structure of neutral aluminum clustersAln(2â©½nâ©½23): Genetic algorithm tight-binding calculations. Physical Review B, 2006, 73, .	1.1	113
21	Laser-Induced Graphitization on a Diamond (111) Surface. Physical Review Letters, 2000, 85, 4092-4095.	2.9	107
22	The geometry of large fullerene cages: C72 to C102. Journal of Chemical Physics, 1993, 98, 3095-3102.	1.2	105
23	Core energy and Peierls stress of a screw dislocation in bcc molybdenum: A periodic-cell tight-binding study. Physical Review B, 2004, 70, .	1.1	105
24	New Layered Structures of Cuprous Chalcogenides as Thin Film Solar Cell Materials:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>Te</mml:mi></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>Se</mml:mi></mml:math>. Physical Review Letters, 2013, 111, 165502.	2.9	103
25	Zero-Strain Na₂FeSiO₄ as Novel Cathode Material for Sodium-Ion Batteries. ACS Applied Materials & Interfaces, 2016, 8, 17233-17238.	4.0	101
26	Interlayer gap widened Î±-phase molybdenum trioxide as high-rate anodes for dual-ion-intercalation energy storage devices. Nature Communications, 2020, 11, 1348.	5.8	100
27	Exploring the Structural Complexity of Intermetallic Compounds by an Adaptive Genetic Algorithm. Physical Review Letters, 2014, 112, 045502.	2.9	97
28	Structures and Fragmentations of Small Silicon Oxide Clusters by ab Initio Calculations. Journal of Physical Chemistry A, 2003, 107, 6936-6943.	1.1	94
29	Quasiatomic orbitals forab initiotight-binding analysis. Physical Review B, 2008, 78, .	1.1	90
30	Vacancy defects and the formation of local haeckelite structures in graphene from tight-binding molecular dynamics. Physical Review B, 2006, 74, .	1.1	81
31	Search for the groundâ€state structure of C84. Journal of Chemical Physics, 1992, 96, 7183-7185.	1.2	72
32	Ultrahigh-pressure phases of H<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>O ice predicted using an adaptive genetic algorithm. Physical Review B, 2011, 84, .	1.1	72
33	Dissociation Energies of Silicon Clusters: A Depth Gauge for the Global Minimum on the Potential Energy Surface. Physical Review Letters, 1998, 81, 4616-4619.	2.9	71
34	Spatially Resolved Distribution Function and the Medium-Range Order in Metallic Liquid and Glass. Scientific Reports, 2011, 1, 194.	1.6	69
35	Experimental and molecular dynamics simulation study of structure of liquid and amorphous Ni62Nb38 alloy. Journal of Chemical Physics, 2016, 145, 204505.	1.2	69
36	Phase Diagram and Electronic Structure of Praseodymium and Plutonium. Physical Review X, 2015, 5, .	2.8	67

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37	Selenium Edge as a Selective Anchoring Site for Lithiumâ€“Sulfur Batteries with MoSe₂/Graphene-Based Cathodes. ACS Applied Materials & Interfaces, 2019, 11, 19986-19993.	4.0	67
38	Adsorption and growth morphology of rare-earth metals on graphene studied byab initiocalculations and scanning tunneling microscopy. Physical Review B, 2010, 82, .	1.1	66
39	Magic Structures of H-Passivated âŒ©110âŒª Silicon Nanowires. Nano Letters, 2006, 6, 277-281.	4.5	65
40	Gutzwiller density functional theory for correlated electron systems. Physical Review B, 2008, 77, .	1.1	65
41	Representation of electronic structures in crystals in terms of highly localized quasiatomic minimal basis orbitals. Physical Review B, 2004, 70, .	1.1	63
42	Development of a semi-empirical potential suitable for molecular dynamics simulation of vitrification in Cu-Zr alloys. Journal of Chemical Physics, 2019, 151, 214502.	1.2	63
43	Development of interatomic potentials appropriate for simulation of devitrification of Al₉₀Sm₁₀alloy. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 045013.	0.8	61
44	Transition metals on the (0 0 0 1) surface of graphite: Fundamental aspects of adsorption, diffusion, and morphology. Progress in Surface Science, 2014, 89, 219-238.	3.8	60
45	Adaptive Variational Quantum Dynamics Simulations. PRX Quantum, 2021, 2, .	3.5	57
46	Atomic size and chemical effects on the local order of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Zr</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub	1.1	55
47	Reconstruction and evaporation at graphene nanoribbon edges. Physical Review B, 2010, 81, .	1.1	55
48	Relationship between structure and conductivity in liquid carbon. Physical Review B, 1995, 52, 4138-4145.	1.1	52
49	Molecule intrinsic minimal basis sets. II. Bonding analyses for Si4H6 and Si2 to Si10. Journal of Chemical Physics, 2004, 120, 2638-2651.	1.2	52
50	â€˜Crystal Genesâ€™ in Metallic Liquids and Glasses. Scientific Reports, 2016, 6, 23734.	1.6	52
51	Effects of sub-Tg annealing on Cu64.5Zr35.5 glasses: A molecular dynamics study. Applied Physics Letters, 2014, 104, .	1.5	51
52	Photodepositing CdS on the Active Cyano Groups Decorated gâ€C₃N₄ in Zâ€Scheme Manner Promotes Visibleâ€Lightâ€Driven Hydrogen Evolution. Small, 2021, 17, e2102699.	5.2	51
53	Melting of small Sn clusters byab initiomolecular dynamics simulations. Physical Review B, 2004, 69, .	1.1	50
54	Finding the low-energy structures of Si[001] symmetric tilted grain boundaries with a genetic algorithm. Physical Review B, 2009, 80, .	1.1	49

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55	Cooling rate dependence of medium-range order development in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>36</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>Zr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	1.1	48
56	Coupling of the dynamics of medium-range order and short-range order in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>64</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>by<i>ab	1.1	47
57	Ferromagnetic Quantum Critical Point Avoided by the Appearance of Another Magnetic Phase in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	2.9	47
58	Pressure. Physical Review Letters, 2016, 117, 037207. Identification of post-pyrite phase transitions in SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	1.1	46
59	Overcoming the Time Limitation in Molecular Dynamics Simulation of Crystal Nucleation: A Persistent-Embryo Approach. Physical Review Letters, 2018, 120, 085703.	2.9	46
60	Large magnetic anisotropy predicted for rare-earth-free <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi	1.1	46
61	Light control of surfaceâ€“bulk coupling by terahertz vibrational coherence in a topological insulator. Npj Quantum Materials, 2020, 5, .	1.8	45
62	Short- and medium-range order in a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	1.1	43
63	Fundamental Link between Î² Relaxation, Excess Wings, and Cage-Breaking in Metallic Glasses. Journal of Physical Chemistry Letters, 2018, 9, 5877-5883.	2.1	44
64	Cooling rate dependence of structural order in Al90Sm10 metallic glass. Journal of Applied Physics, 2016, 120, .	1.1	43
65	Tailoring Bandgap of Perovskite BaTiO3 by Transition Metals Co-Doping for Visible-Light Photoelectrical Applications: A First-Principles Study. Nanomaterials, 2018, 8, 455.	1.9	42
66	Efficient Step-Merged Quantum Imaginary Time Evolution Algorithm for Quantum Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 6256-6266.	2.3	42
67	Highly localized quasiatomic minimal basis orbitals for Mo fromab initiocalculations. Physical Review B, 2007, 76, .	1.1	41
68	Interface Structure Prediction from First-Principles. Journal of Physical Chemistry C, 2014, 118, 9524-9530.	1.5	39
69	Electrochemical and density functional theory investigation on the differential behaviors of core-ring structured NiCo 2 O 4 nanoplatelets toward heavy metal ions. Analytica Chimica Acta, 2018, 1022, 37-44.	2.6	39
70	Development of a deep machine learning interatomic potential for metalloid-containing Pd-Si compounds. Physical Review B, 2019, 100, .	1.1	39
71	Short- and medium-range order in amorphous<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" alloy. Physical Review B, 2010, 81, .	1.1	38
72	Growth morphology and thermal stability of metal islands on graphene. Physical Review B, 2012, 86, .	1.1	38

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73	Evolution of short- and medium-range order in the melt-quenching amorphization of Ge₂Sb₂Te₅. Journal of Materials Chemistry C, 2018, 6, 5001-5011.	2.7	38
74	Predicting Complex Relaxation Processes in Metallic Glass. Physical Review Letters, 2019, 123, 105701.	2.9	36
75	Quantum Size Effects in the Growth, Coarsening, andÂProperties of Ultra-thin Metal Films andÂRelatedÂNanostructures. Journal of Low Temperature Physics, 2009, 157, 221-251.	0.6	35
76	Vibrational modes and lattice distortion of a nitrogen-vacancy center in diamond from first-principles calculations. Physical Review B, 2011, 84, .	1.1	35
77	Interface mobility and the liquid-glass transition in a one-component system described by an embedded atom method potential. Physical Review B, 2006, 74, .	1.1	34
78	The formation of pentagon-heptagon pair defect by the reconstruction of vacancy defects in carbon nanotube. Applied Physics Letters, 2008, 92, 043104.	1.5	33
79	Structural signature and transition dynamics of Sb₂Te₃ melt upon fast cooling. Physical Chemistry Chemical Physics, 2018, 20, 11768-11775.	1.3	33
80	Transforming Photocatalytic gâ€C₃N₄/MoSe₂ into a Direct Zâ€Scheme System via Boronâ€Doping: A Hybrid DFT Study. ChemSusChem, 2020, 13, 4985-4993.	3.6	33
81	Formation of carbon nanotube semiconductor-metal intramolecular junctions by self-assembly of vacancy defects. Physical Review B, 2007, 76, .	1.1	32
82	Molecular dynamics investigation of dynamical heterogeneity and local structure in the supercooled liquid and glass states of Al. Physical Review B, 2008, 77, .	1.1	32
83	Adaptive Variational Quantum Imaginary Time Evolution Approach for Ground State Preparation. Advanced Quantum Technologies, 2021, 4, 2100114.	1.8	32
84	Formation and development of dislocation in graphene. Applied Physics Letters, 2013, 102, .	1.5	31
85	Comparing efficiencies of genetic and minima hopping algorithms for crystal structure prediction. Physical Chemistry Chemical Physics, 2010, 12, 11617.	1.3	30
86	Structural and dynamical properties of liquid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Cu</mml:mi><mml:mrow><mml:mn>80</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">Si</mml:mi><mml:mrow><mml:mn>20</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>alloy studied experimentally and by<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="italic">ab</mml:mi>. Physical Review B, 2011, 84, .	1.1	29
87	Unique Dynamic Appearance of a Ge-Si Ad-dimer on Si(001). Physical Review Letters, 2000, 85, 5603-5606.	2.9	28
88	Structures and magnetic properties of Fe clusters on graphene. Physical Review B, 2014, 90, .	1.1	28
89	Metastable cobalt nitride structures with high magnetic anisotropy for rare-earth free magnets. Physical Chemistry Chemical Physics, 2016, 18, 31680-31690.	1.3	28
90	Understanding CrGeTe₃: an abnormal phase change material with inverse resistance and density contrast. Journal of Materials Chemistry C, 2019, 7, 9025-9030.	2.7	28

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91	Development of interatomic potential for Alâ€“Tb alloys using a deep neural network learning method. Physical Chemistry Chemical Physics, 2020, 22, 18467-18479.	1.3	28
92	Topochemical Deintercalation of Li from Layered LiNiB: toward 2D MBene. Journal of the American Chemical Society, 2021, 143, 4213-4223.	6.6	28
93	Transferability of the Slater-Koster tight-binding scheme from an environment-dependent minimal-basis perspective. Physical Review B, 2005, 72, .	1.1	27
94	Directed assembly of Ru nanoclusters on Ru(0001)-supported graphene: STM studies and atomistic modeling. Physical Review B, 2012, 86, .	1.1	27
95	Feâ€“Si networks in Na₂FeSiO₄ cathode materials. Physical Chemistry Chemical Physics, 2016, 18, 23916-23922.	1.3	27
96	Formation of Multilayer Cu Islands Embedded beneath the Surface of Graphite: Characterization and Fundamental Insights. Journal of Physical Chemistry C, 2018, 122, 4454-4469.	1.5	27
97	Comparative study of the electronic and magnetic properties of BaFe<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>As<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>and BaMn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	26
98	Local structure order in Pd78Cu6Si16 liquid. Scientific Reports, 2015, 5, 8277.	1.6	26
99	Manipulation of Dirac cones in intercalated epitaxial graphene. Carbon, 2017, 123, 93-98.	5.4	25
100	A deep learning interatomic potential developed for atomistic simulation of carbon materials. Carbon, 2022, 186, 1-8.	5.4	25
101	Competition between fcc and icosahedral short-range orders in pure and samarium-doped liquid aluminum from first principles. Physical Review B, 2011, 83, .	1.1	24
102	Defect-mediated, thermally-activated encapsulation of metals at the surface of graphite. Carbon, 2018, 127, 305-311.	5.4	24
103	Multilayered metal-dielectric film structure for highly efficient solar selective absorption. Materials Research Express, 2018, 5, 066428.	0.8	24
104	Magnetism of new metastable cobalt-nitride compounds. Nanoscale, 2018, 10, 13011-13021.	2.8	24
105	Computationally Driven Discovery of a Family of Layered LiNiB Polymorphs. Angewandte Chemie - International Edition, 2019, 58, 15855-15862.	7.2	24
106	Shallow-circuit variational quantum eigensolver based on symmetry-inspired Hilbert space partitioning for quantum chemical calculations. Physical Review Research, 2021, 3, .	1.3	24
107	Fe-Fe adatom interaction and growth morphology on graphene. Physical Review B, 2011, 84, .	1.1	23
108	A first-principles study of Group IV dimer chains on Si(100). Physical Review B, 2005, 72, .	1.1	21

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109	Magnetocrystalline anisotropy in cobalt based magnets: a choice of correlation parameters and the relativistic effects. Journal of Physics Condensed Matter, 2018, 30, 195801.	0.7	21
110	Gutzwiller hybrid quantum-classical computing approach for correlated materials. Physical Review Research, 2021, 3, .	1.3	21
111	Honeycomb chain structure of theAuâ•Si(111)â˜(5Ã—2)surface reconstruction: A first-principles study. Physical Review B, 2008, 77, .	1.1	20
112	Including many-body screening into self-consistent calculations: Tight-binding model studies with the Gutzwiller approximation. Physical Review B, 2011, 83, .	1.1	20
113	Structures and stabilities of alkaline earth metal peroxides XO2 (X = Ca, Be, Mg) studied by a genetic algorithm. RSC Advances, 2013, 3, 22135.	1.7	20
114	Interplay of spin-orbit and entropic effects in cerium. Physical Review B, 2014, 90, .	1.1	20
115	Electrochemically self-doped hierarchical TiO₂ nanotube arrays for enhanced visible-light photoelectrochemical performance: an experimental and computational study. RSC Advances, 2016, 6, 46871-46878.	1.7	20
116	Local structure origin of ultrafast crystallization driven by high-fidelity octahedral clusters in amorphous Sc0.2Sb2Te3. Applied Physics Letters, 2019, 114, .	1.5	20
117	Model reconstructions for the Si(337) orientation. Journal of Applied Physics, 2005, 98, 073507.	1.1	19
118	Atomic structure and magnetic properties of Fe1â€“xCox alloys. Journal of Applied Physics, 2012, 111, 07E338.	1.1	19
119	Cooling rate dependence of structural order in Ni62Nb38 metallic glass. Journal of Applied Physics, 2018, 123, 045108.	1.1	19
120	Tailored Plasmons in Pentacene/Graphene Heterostructures with Interlayer Electron Transfer. Nano Letters, 2019, 19, 6058-6064.	4.5	19
121	From NaZn₄Sb₃ to HT-Na_{1â€“x}Zn_{4â€“y}Sb₃: Panoramic Hydride Synthesis, Structural Diversity, and Thermoelectric Properties. Chemistry of Materials, 2019, 31, 8695-8707.	3.2	19
122	Tight-Binding Molecular Dynamics Studies of Covalent Systems. Advances in Chemical Physics, 2007, , 651-702.	0.3	18
123	Effects of Oxygen Impurities on Glass-Formation Ability in Zr₂Cu Alloy. Journal of Physical Chemistry B, 2016, 120, 9223-9229.	1.2	18
124	Structural ordering at solid-liquid interfaces in Al-Sm system: A molecular-dynamics study. Materials Letters, 2017, 186, 26-29.	1.3	18
125	Material simulations with tight-binding molecular dynamics. Journal of Phase Equilibria and Diffusion, 1997, 18, 516-529.	0.3	17
126	Double icosahedronâ€based motif of Ni_n (n = 20â˜30). International Journal of Quantum Chemistry, 2012, 112, 1717-1724.	1.0	17

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127	Three-center tight-binding potential model for C and Si. Physical Review B, 2015, 92, .	1.1	17
128	Tight-binding calculation studies of vacancy and adatom defects in graphene. Journal of Physics Condensed Matter, 2016, 28, 115001.	0.7	17
129	Temperature dependence of the solid-liquid interface free energy of Ni and Al from molecular dynamics simulation of nucleation. Journal of Chemical Physics, 2018, 149, 174501.	1.2	17
130	Nucleation of stoichiometric compounds from liquid: Role of the kinetic factor. Physical Review Materials, 2018, 2, .	0.9	17
131	Fluctuation between icosahedral and body-centered-cube short-range orders in undercooled Zr liquid. Journal of Applied Physics, 2011, 110, .	1.1	16
132	Topological states in A15 superconductors. Physical Review B, 2019, 99, .	1.1	16
133	Formation criterion for binary metal diboride solid solutions established through combinatorial methods. Journal of the American Ceramic Society, 2020, 103, 3338-3348.	1.9	16
134	The role of pentagonâ€“heptagon pair defect in carbon nanotube: The center of vacancy reconstruction. Applied Physics Letters, 2010, 97, 093106.	1.5	15
135	Nonclassical â€œExplosiveâ€•Nucleation in Pb/Si(111) at Low Temperatures. Physical Review Letters, 2014, 113, 236101.	2.9	15
136	Determining whether metals nucleate homogeneously on graphite: A case study with copper. Physical Review B, 2014, 90, .	1.1	15
137	Correlation matrix renormalization approximation for total-energy calculations of correlated electron systems. Physical Review B, 2014, 89, .	1.1	15
138	Structures and magnetic properties of Co-Zr-B magnets studied by first-principles calculations. Journal of Applied Physics, 2015, 117, .	1.1	15
139	Unraveling the structural and bonding nature of antimony sesquichalcogenide glass for electronic and photonic applications. Journal of Materials Chemistry C, 0, , .	2.7	15
140	Structure, bonding nature and transition dynamics of amorphous Te. Scripta Materialia, 2021, 202, 114011.	2.6	15
141	Third time's the charm: intricate non-centrosymmetric polymorphism in LnSiP₃ (Ln = La and Ce) induced by distortions of phosphorus square layers. Dalton Transactions, 2021, 50, 6463-6476.	1.6	15
142	Melting of carbon cages. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 285-287.	1.0	14
143	Evolution of optical properties of tin film from solid to liquid studied by spectroscopic ellipsometry and ab initio calculation. Applied Physics Letters, 2014, 104, 121907.	1.5	14
144	Structures and stability of metal-doped GenM (n = 9, 10) clusters. AIP Advances, 2015, 5, .	0.6	14

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145	Correlation Matrix Renormalization Theory: Improving Accuracy with Two-Electron Density-Matrix Sum Rules. Journal of Chemical Theory and Computation, 2016, 12, 4806-4811.	2.3	14
146	Polyamorphism in K₂Sb₈Se₁₃ for multi-level phase-change memory. Journal of Materials Chemistry C, 2020, 8, 6364-6369.	2.7	14
147	Structural hierarchy as a key to complex phase selection in Al-Sm. Physical Review Materials, 2017, 1, .	0.9	14
148	Medium-range icosahedral order in quasicrystal-forming Zr2Pd binary metallic glass. Applied Physics Letters, 2011, 98, .	1.5	13
149	Impact of deformation on the atomic structures and dynamics of a Cu-Zr metallic glass: A molecular dynamics study. Physical Review B, 2014, 90, .	1.1	13
150	Discovery of a meta-stable Alâ€“Sm phase with unknown stoichiometry using a genetic algorithm. Scripta Materialia, 2014, 81, 32-35.	2.6	13
151	Synergistic computational and experimental discovery of novel magnetic materials. Molecular Systems Design and Engineering, 2020, 5, 1098-1117.	1.7	13
152	Mechanism of Metal Intercalation under Graphene through Small Vacancy Defects. Journal of Physical Chemistry C, 2021, 125, 6954-6962.	1.5	13
153	Ultrafast crystallization mechanism of amorphous Ge15Sb85 unraveled by pressure-driven simulations. Acta Materialia, 2021, 216, 117123.	3.8	13
154	Competition between area and height evolution of Pb islands on a Si(111) surface. Physical Review B, 2009, 79, .	1.1	12
155	Feâ€“Si networks and charge/discharge-induced phase transitions in Li₂FeSiO₄ cathode materials. Physical Chemistry Chemical Physics, 2018, 20, 14557-14563.	1.3	12
156	Structural features of chalcogenide glass SiTe: An ovonic threshold switching material. APL Materials, 2021, 9, .	2.2	12
157	Efficient and accurate treatment of electron correlations with Correlation Matrix Renormalization theory. Scientific Reports, 2015, 5, 13478.	1.6	11
158	A computational study of diffusion in a glass-forming metallic liquid. Scientific Reports, 2015, 5, 10956.	1.6	11
159	Crystal structure and magnetic properties of new Fe₃Co₃X₂(Xâ€‰â€‰=â€‰â€‰Ti, Nb) intermetallic compounds. Journal Physics D: Applied Physics, 2016, 49, 175002.	1.3	11
160	Exploring new phases of Fe_{3â^’x}Co_xC for rare-earth-free magnets. Journal Physics D: Applied Physics, 2017, 50, 215005.	1.3	11
161	Manipulation of electronic property of epitaxial graphene on SiC substrate by Pb intercalation. Physical Review B, 2021, 103, .	1.1	11
162	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	0.9	11

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163	Structures ofSi7H2m(m=1â€“7)clusters by global optimization. Physical Review B, 2006, 74, .	1.1	10
164	Theoretical Prediction of Si₂â€“Si₃₃ Absorption Spectra. Journal of Physical Chemistry A, 2017, 121, 6388-6397.	1.1	10
165	Effects of Si solute on the glass formation and atomic structure of Pd liquid. Journal of Physics Condensed Matter, 2019, 31, 135701.	0.7	10
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