Cai-Zhuang Wang

List of Publications by Year
in descending order

285 papers	9,953 citations	38738 50 h-index	46795 89 g-index
299 all docs	299 docs citations	299 times ranked	9421 citing authors

#	Article	IF	Citations
1	A deep learning interatomic potential developed for atomistic simulation of carbon materials. Carbon, 2022, 186, 1-8.	10.3	25
2	Neural network potential for Zrâ€“Rh system by machine learning. Journal of Physics Condensed Matter, 2022, 34, 075402.	1.8	6
3	Predicting magnetic anisotropy energies using site-specific spin-orbit coupling energies and machine learning: Application to iron-cobalt nitrides. Physical Review Materials, 2022, 6, .	2.4	3
4	Straintronic Effect on Phonon-Mediated Superconductivity of Nb₂CT₂ (T = O,) Tj ETQq0 0 0 rgBT /Overlock 10	3.1	5
5	Reversible motions and disordered structure of soft particles in amorphous solids. Physical Review B, 2022, 105, .	3.2	0
6	Highly Asymmetric Graphene Layer Doping and Band Structure Manipulation in Rare Earthâ€“Graphene Heterostructure by Targeted Bonding of the Intercalated Gadolinium. Journal of Physical Chemistry C, 2022, 126, 6863-6873.	3.1	10
7	The Gutzwiller conjugate gradient minimization method for correlated electron systems. Journal of Physics Condensed Matter, 2022, 34, 243001.	1.8	4
8	Structure and motifs of iron oxides from 1 to 3 TPa. Physical Review Materials, 2022, 6, .	2.4	1
9	Deep machine learning potential for atomistic simulation of Fe-Si-O systems under Earth's outer core conditions. Physical Review Materials, 2022, 6, .	2.4	8
10	Ground state wave functions for single-band Hubbard models from the Gutzwiller conjugate gradient minimisation theory. Molecular Physics, 2021, 119, e1797917.	1.7	5
11	An efficient random-sampling method for calculating double occupancy of Gutzwiller wave function in single-band 1D and 2D lattices. Molecular Physics, 2021, 119, e1812745.	1.7	3
12	Luminescence mechanism in hydrogenated silicon quantum dots with a single oxygen ligand. Nanoscale Advances, 2021, 3, 2245-2251.	4.6	5
13	Shallow-circuit variational quantum eigensolver based on symmetry-inspired Hilbert space partitioning for quantum chemical calculations. Physical Review Research, 2021, 3, .	3.6	24
14	Crystallization of the P₃Sn₄ Phase upon Cooling P₂Sn₅ Liquid by Molecular Dynamics Simulation Using a Machine Learning Interatomic Potential. Journal of Physical Chemistry C, 2021, 125, 3127-3133.	3.1	7
15	Localized electronic and vibrational states in amorphous diamond. Physical Chemistry Chemical Physics, 2021, 23, 4835-4840.	2.8	2
16	Lithium nickel borides: evolution of [NiB] layers driven by Li pressure. Inorganic Chemistry Frontiers, 2021, 8, 1675-1685.	6.0	7
17	Characterizations of electronic and optical properties of Sb-based phase-change material stabilized by alloying Cr. Applied Physics Letters, 2021, 118, .	3.3	7
18	Encapsulation of metal nanoparticles at the surface of a prototypical layered material. Nanoscale, 2021, 13, 1485-1506.	5.6	10

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19	Gutzwiller hybrid quantum-classical computing approach for correlated materials. Physical Review Research, 2021, 3, .	3.6	21
20	Manipulation of electronic property of epitaxial graphene on SiC substrate by Pb intercalation. Physical Review B, 2021, 103, .	3.2	11
21	Evidence for a large Rashba splitting in PtPb4 from angle-resolved photoemission spectroscopy. Physical Review B, 2021, 103, .	3.2	3
22	Mechanism of Metal Intercalation under Graphene through Small Vacancy Defects. Journal of Physical Chemistry C, 2021, 125, 6954-6962.	3.1	13
23	Topochemical Deintercalation of Li from Layered LiNiB: toward 2D MBene. Journal of the American Chemical Society, 2021, 143, 4213-4223.	13.7	28
24	Unveiling the mechanism of phase and morphology selections during the devitrification of Al-Sm amorphous ribbon. Physical Review Materials, 2021, 5, .	2.4	3
25	Nonequilibrium phonon tuning and mapping in few-layer graphene with infrared nanoscopy. Physical Review B, 2021, 103, .	3.2	7
26	Adaptive Variational Quantum Dynamics Simulations. PRX Quantum, 2021, 2, .	9.2	57
27	Role of Coulomb interaction in the phase formation of fcc Ce: Correlation matrix renormalization theory. Physical Review B, 2021, 104, .	3.2	6
28	Photodepositing CdS on the Active Cyano Groups Decorated gâ€C‹sub›3‹/sub›N‹sub›4‹/sub› in Zâ€Scheme Manner Promotes Visibleâ€Lightâ€Driven Hydrogen Evolution. Small, 2021, 17, e2102699.	10.0	51
29	Structural features of chalcogenide glass SiTe: An ovonic threshold switching material. APL Materials, 2021, 9, .	5.1	12
30	Structure, bonding nature and transition dynamics of amorphous Te. Scripta Materialia, 2021, 202, 114011.	5.2	15
31	Ultrafast crystallization mechanism of amorphous Ge15Sb85 unraveled by pressure-driven simulations. Acta Materialia, 2021, 216, 117123.	7.9	13
32	Magnetism and topological Hall effect in antiferromagnetic Ru2MnSn-based Heusler compounds. Journal of Magnetism and Magnetic Materials, 2021, 537, 168104.	2.3	5
33	Third time's the charm: intricate non-centrosymmetric polymorphism in ‹i›Ln‹/i›SiP‹sub›3‹/sub› (‹i›Ln‹/i› = La and Ce) induced by distortions of phosphorus square layers. Dalton Transactions, 2021, 50, 6463-6476.	3.3	15
34	Correlation matrix renormalization theory in multi-band lattice systems. Journal of Physics Condensed Matter, 2021, 33, 095902.	1.8	3
35	Adaptive Variational Quantum Imaginary Time Evolution Approach for Ground State Preparation. Advanced Quantum Technologies, 2021, 4, 2100114.	3.9	32
36	Unconventional iron-magnesium compounds at terapascal pressures. Physical Review B, 2021, 104, .	3.2	3

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37	Molecular dynamics simulation of metallic Alâ€“Ce liquids using a neural network machine learning interatomic potential. Journal of Chemical Physics, 2021, 155, 194503.	3.0	9
38	Pressure-induced superconductivity in the hydrogen-rich pseudobinary CaBâ‚Hn compounds. Physical Review B, 2021, 104, .	3.2	5
39	Lithium Diffusion in Silicon Encapsulated with Graphene. Nanomaterials, 2021, 11, 3397.	4.1	3
40	Defect Interaction and Deformation in Graphene. Journal of Physical Chemistry C, 2020, 124, 2370-2378.	3.1	6
41	Formation criterion for binary metal diboride solid solutions established through combinatorial methods. Journal of the American Ceramic Society, 2020, 103, 3338-3348.	3.8	16
42	Efficient Step-Merged Quantum Imaginary Time Evolution Algorithm for Quantum Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 6256-6266.	5.3	42
43	Transforming Photocatalytic gâ€C₃N₄/MoSe₂ into a Direct Zâ€Scheme System via Boronâ€Doping: A Hybrid DFT Study. ChemSusChem, 2020, 13, 4985-4993.	6.8	33
44	Development of interatomic potential for Alâ€“Tb alloys using a deep neural network learning method. Physical Chemistry Chemical Physics, 2020, 22, 18467-18479.	2.8	28
45	A benchmark of Gutzwiller conjugate gradient minimization method in ground state energy calculations of dimers. Computational and Theoretical Chemistry, 2020, 1185, 112877.	2.5	4
46	Dynamic Observation of Dendritic Quasicrystal Growth upon Laser-Induced Solid-State Transformation. Physical Review Letters, 2020, 125, 195503.	7.8	7
47	Spatial decomposition of magnetic anisotropy in magnets: Application to doped Fe16N2. Physical Review B, 2020, 102, .	3.2	8
48	Phase Diagram and Structure Map of Binary Nanoparticle Superlattices from a Lennard-Jones Model. ACS Nano, 2020, 14, 6795-6802.	14.6	9
49	Stabilizing the crystal structures of NaFePO₄ with Li substitutions. Physical Chemistry Chemical Physics, 2020, 22, 13975-13980.	2.8	8
50	Ground-state properties of the Hubbard model in one and two dimensions from the Gutzwiller conjugate gradient minimization theory. Physical Review B, 2020, 101, .	3.2	7
51	Synergistic computational and experimental discovery of novel magnetic materials. Molecular Systems Design and Engineering, 2020, 5, 1098-1117.	3.4	13
52	Unveiling the medium-range order in glass models and its role in glass formation. Physical Review B, 2020, 101, .	3.2	5
53	Characterization of three phases of liquid carbon by tight-binding molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 14630-14636.	2.8	4
54	Interlayer gap widened Î±-phase molybdenum trioxide as high-rate anodes for dual-ion-intercalation energy storage devices. Nature Communications, 2020, 11, 1348.	12.8	100

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55	Theoretical search for possible Liâ€“Niâ€“B crystal structures using an adaptive genetic algorithm. Journal of Applied Physics, 2020, 127, .	2.5	8
56	Light control of surfaceâ€“bulk coupling by terahertz vibrational coherence in a topological insulator. Npj Quantum Materials, 2020, 5, .	5.2	45
57	First-principles calculation of excited states of diatomic molecules: a benchmark for the Gutzwiller conjugate gradient minimisation method. Molecular Physics, 2020, 118, .	1.7	6
58	Polyamorphism in K₂Sb₈Se₁₃ for multi-level phase-change memory. Journal of Materials Chemistry C, 2020, 8, 6364-6369.	5.5	14
59	Origin of short- and medium-range order in supercooled liquid Ge₃Sb₂Te₆ using ab initio molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 9759-9766.	2.8	4
60	Electronic Structure of Double-Layer Epitaxial Graphene on SiC(0001) Modified by Gd Intercalation. Journal of Physical Chemistry C, 2020, 124, 28132-28138.	3.1	8
61	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	2.4	11
62	Adaptive Genetic Algorithm for Structure Prediction and Application to Magnetic Materials. , 2020, , 2757-2776.		0
63	Tailored Plasmons in Pentacene/Graphene Heterostructures with Interlayer Electron Transfer. Nano Letters, 2019, 19, 6058-6064.	9.1	19
64	Computationally Driven Discovery of a Family of Layered LiNiB Polymorphs. Angewandte Chemie, 2019, 131, 16002-16009.	2.0	5
65	First-principles calculation of correlated electron materials based on Gutzwiller wave function beyond Gutzwiller approximation. Journal of Physics Condensed Matter, 2019, 31, 335601.	1.8	8
66	Computationally Driven Discovery of a Family of Layered LiNiB Polymorphs. Angewandte Chemie - International Edition, 2019, 58, 15855-15862.	13.8	24
67	Understanding CrGeTe₃: an abnormal phase change material with inverse resistance and density contrast. Journal of Materials Chemistry C, 2019, 7, 9025-9030.	5.5	28
68	Temperature dependence of structural, dynamical, and electronic properties of amorphous Bi₂Te₃: an ab initio study. New Journal of Physics, 2019, 21, 093062.	2.9	4
69	Development of a deep machine learning interatomic potential for metalloid-containing Pd-Si compounds. Physical Review B, 2019, 100, .	3.2	39
70	Predicting Complex Relaxation Processes in Metallic Glass. Physical Review Letters, 2019, 123, 105701.	7.8	36
71	Strong optical absorption of a metallic film to induce a lensing effect in the visible region. Scientific Reports, 2019, 9, 12434.	3.3	1
72	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.	6.7	19

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73	Observation of Î·-Al41Sm5 reveals motif-aware structural evolution in Al-Sm alloys. Scientific Reports, 2019, 9, 6692.	3.3	4
74	Quantum phase transition and ferromagnetism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">o</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>+</mml:mo><mml:mi>x</mml:mi></mml:mrow></m Physical Review B, 2019, 99, .	3.2	4
75	Topological states in A15 superconductors. Physical Review B, 2019, 99, .	3.2	16
76	Selenium Edge as a Selective Anchoring Site for Lithiumâ€“Sulfur Batteries with MoSe₂/Graphene-Based Cathodes. ACS Applied Materials & Interfaces, 2019, 11, 19986-19993.	8.0	67
77	Benchmark of correlation matrix renormalization method in molecule calculations. Journal of Physics Condensed Matter, 2019, 31, 195902.	1.8	2
78	Competitive B2 and B33 Nucleation during Solidification of Ni50Zr50 Alloy: Molecular Dynamics Simulation and Classical Nucleation Theory. Journal of Physical Chemistry C, 2019, 123, 6685-6692.	3.1	6
79	Local structure origin of ultrafast crystallization driven by high-fidelity octahedral clusters in amorphous Sc0.2Sb2Te3. Applied Physics Letters, 2019, 114, .	3.3	20
80	Development of a semi-empirical potential suitable for molecular dynamics simulation of vitrification in Cu-Zr alloys. Journal of Chemical Physics, 2019, 151, 214502.	3.0	63
81	Adaptive Genetic Algorithm for Structure Prediction and Application to Magnetic Materials. , 2019, , 1-20.		1
82	Thermal conductivity of TiO2 nanotube: a molecular dynamics study. Journal of Physics Condensed Matter, 2019, 31, 055302.	1.8	4
83	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.	3.8	217
84	Effects of Si solute on the glass formation and atomic structure of Pd liquid. Journal of Physics Condensed Matter, 2019, 31, 135701.	1.8	10
85	Effects of dopants on the glass forming ability in Al-based metallic alloy. Physical Review Materials, 2019, 3, .	2.4	10
86	Microstructure evolution during near- Tg annealing and its effect on shear banding in model alloys. Physical Review Materials, 2019, 3, .	2.4	3
87	Correlation matrix renormalization theory for correlated-electron materials with application to the crystalline phases of atomic hydrogen. Physical Review B, 2018, 97, .	3.2	7
88	Overcoming the Time Limitation in Molecular Dynamics Simulation of Crystal Nucleation: A Persistent-Embryo Approach. Physical Review Letters, 2018, 120, 085703.	7.8	46
89	Ternary Bismuthide SrPtBi₂: Computation and Experiment in Synergism to Explore Solid-State Materials. Journal of Physical Chemistry C, 2018, 122, 5057-5063.	3.1	4
90	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.	5.4	39

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91	Magnetocrystalline anisotropy in cobalt based magnets: a choice of correlation parameters and the relativistic effects. Journal of Physics Condensed Matter, 2018, 30, 195801.	1.8	21
92	A comparative study of Sm networks in Al-10 at.%Sm glass and associated crystalline phases. Philosophical Magazine Letters, 2018, 98, 27-37.	1.2	2
93	Evolution of short- and medium-range order in the melt-quenching amorphization of Ge₂Sb₂Te₅. Journal of Materials Chemistry C, 2018, 6, 5001-5011.	5.5	38
94	Formation of Multilayer Cu Islands Embedded beneath the Surface of Graphite: Characterization and Fundamental Insights. Journal of Physical Chemistry C, 2018, 122, 4454-4469.	3.1	27
95	Cooling rate dependence of structural order in Ni62Nb38 metallic glass. Journal of Applied Physics, 2018, 123, 045108.	2.5	19
96	New structures of Fe₃S for rare-earth-free permanent magnets. Journal Physics D: Applied Physics, 2018, 51, 075001.	2.8	4
97	Feâ€“Si networks and charge/discharge-induced phase transitions in Li₂FeSiO₄ cathode materials. Physical Chemistry Chemical Physics, 2018, 20, 14557-14563.	2.8	12
98	Using first-principles calculations to screen for fragile magnetism: Case study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">LaCrGe</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">LaCrSb</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2018, 97, .	3.2	6
99	Structural signature and transition dynamics of Sb₂Te₃ melt upon fast cooling. Physical Chemistry Chemical Physics, 2018, 20, 11768-11775.	2.8	33
100	Investigation of partitionless growth ofÎµ-Al₆₀Sm₁₁phase in Al-10 at% Sm liquid. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 015006.	2.0	7
101	Defect-mediated, thermally-activated encapsulation of metals at the surface of graphite. Carbon, 2018, 127, 305-311.	10.3	24
102	Calculation of critical nucleation rates by the persistent embryo method: application to quasi hard sphere models. Soft Matter, 2018, 14, 9185-9193.	2.7	5
103	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.	3.0	17
104	Fundamental Link between Î² Relaxation, Excess Wings, and Cage-Breaking in Metallic Glasses. Journal of Physical Chemistry Letters, 2018, 9, 5877-5883.	4.6	44
105	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.	21.0	244
106	Multilayered metal-dielectric film structure for highly efficient solar selective absorption. Materials Research Express, 2018, 5, 066428.	1.6	24
107	Effect of samarium doping on the nucleation of fcc-aluminum in undercooled liquids. Scripta Materialia, 2018, 154, 202-206.	5.2	5
108	Tailoring Bandgap of Perovskite BaTiO3 by Transition Metals Co-Doping for Visible-Light Photoelectrical Applications: A First-Principles Study. Nanomaterials, 2018, 8, 455.	4.1	42

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109	Structures and magnetic properties of iron silicide from adaptive genetic algorithm and first-principles calculations. Journal of Applied Physics, 2018, 124, .	2.5	6
110	Magnetism of new metastable cobalt-nitride compounds. Nanoscale, 2018, 10, 13011-13021.	5.6	24
111	Nucleation of stoichiometric compounds from liquid: Role of the kinetic factor. Physical Review Materials, 2018, 2, .	2.4	17
112	Influence of nitrogen dopants on the magnetization of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Co</mml:mi><mml:mn>3</mml:mn></mml: mathvariant="normal">N</mml:mi></mml:mrow></mml:math> clusters. Physical Review Materials, 2018, 2,	2.4	7
113	Magnetocrystalline anisotropy in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mrow><mml:mn>64.5</mml:mn></mml:mrow></mml:msub><mml:mi	2.4	7
114	Magnetocrystalline anisotropy in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>YCo</mml:mi><mml:mn>5</mml:mn></mml:msub></mm and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZrCo</mml:mi><mml:mn>5</mml:mn></mml:msub></mm compounds from first-principles real-space pseudopotentials calculations. Physical Review Materials, 2018, 2, .	2.4	4
115	Hybrid siliconâ€“carbon nanostructures for broadband optical absorption. RSC Advances, 2017, 7, 8070-8076.	3.6	5
116	Exploring new phases of Fe_{3â¯'x}Co_xC for rare-earth-free magnets. Journal Physics D: Applied Physics, 2017, 50, 215005.	2.8	11
117	A scheme for the generation of Feâ€“P networks to search for low-energy LiFePO4 crystal structures. Journal of Materials Chemistry A, 2017, 5, 14611-14618.	10.3	9
118	Tuning Cd adsorption behaviours on graphene by introducing defects: a first-principles study. Materials Technology, 2017, 32, 840-844.	3.0	8
119	High photon-to-heat conversion efficiency in the wavelength region of 250â€“1200â€‰nm based on a thermoelectric Bi2Te3 film structure. Scientific Reports, 2017, 7, 44614.	3.3	7
120	Oscillatory electrostatic potential on graphene induced by group IV element decoration. Scientific Reports, 2017, 7, 13152.	3.3	4
121	Growth and characterization of BaZnGa. Philosophical Magazine, 2017, 97, 3317-3324.	1.6	0
122	Transition metal partially supported graphene: Magnetism and oscillatory electrostatic potentials. Journal of Applied Physics, 2017, 122, .	2.5	2
123	Si-centered capped trigonal prism ordering in liquid Pd₈₂Si₁₈ alloy study by first-principles calculations. RSC Advances, 2017, 7, 18093-18098.	3.6	9
124	Structures, phase transitions, and magnetic properties of Co3Si from first-principles calculations. Physical Review B, 2017, 96, .	3.2	8
125	Fe-Cluster Compounds of Chalcogenides: Candidates for Rare-Earth-Free Permanent Magnet and Magnetic Nodal-Line Topological Material. Inorganic Chemistry, 2017, 56, 14577-14583.	4.0	4
126	Cluster-Expansion Model for Complex Quinary Alloys: Application to Alnico Permanent Magnets. Physical Review Applied, 2017, 8, .	3.8	7

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127	Theoretical Prediction of Si₂â€“Si₃₃ Absorption Spectra. Journal of Physical Chemistry A, 2017, 121, 6388-6397.	2.5	10
128	Manipulation of Dirac cones in intercalated epitaxial graphene. Carbon, 2017, 123, 93-98.	10.3	25
129	Theoretical search for possible Au-Si crystal structures using a genetic algorithm. Physical Review B, 2017, 95, .	3.2	9
130	Structural ordering at solid-liquid interfaces in Al-Sm system: A molecular-dynamics study. Materials Letters, 2017, 186, 26-29.	2.6	18
131	Formation of dysprosium carbide on the graphite (0001) surface. Physical Review Materials, 2017, 1, .	2.4	3
132	Structural hierarchy as a key to complex phase selection in Al-Sm. Physical Review Materials, 2017, 1, .	2.4	14
133	Growth mode and structures of magnetic Mn clusters on graphene. RSC Advances, 2016, 6, 64595-64604.	3.6	7
134	Simulations of enhance broadband optical absorption by tuning mie resonance in silicon nanocone arrays. , 2016, , .		0
135	Structure and magnetism of new rare-earth-free intermetallic compounds: Fe3+xCo3â^'xTi2 (0 â‰¤ x â‰¤ 3). APL Materials, 2016, 4, .	5.1	8
136	Adsorption of dysprosium on the graphite (0001) surface: Nucleation and growth at 300 K. Journal of Chemical Physics, 2016, 145, 211902.	3.0	9
137	Experimental and molecular dynamics simulation study of structure of liquid and amorphous Ni62Nb38 alloy. Journal of Chemical Physics, 2016, 145, 204505.	3.0	69
138	Large magnetic anisotropy predicted for rare-earth-free <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">F</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mrow><mml:mn>16</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">o</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:msub><mml:mi mathvariant=	3.2	46
139	Metal intercalation-induced selective adatom mass transport on graphene. Nano Research, 2016, 9, 1434-1441.	10.4	7
140	Electrochemically self-doped hierarchical TiO₂ nanotube arrays for enhanced visible-light photoelectrochemical performance: an experimental and computational study. RSC Advances, 2016, 6, 46871-46878.	3.6	20
141	Feâ€“Si networks in Na₂FeSiO₄ cathode materials. Physical Chemistry Chemical Physics, 2016, 18, 23916-23922.	2.8	27
142	Effects of Oxygen Impurities on Glass-Formation Ability in Zr₂Cu Alloy. Journal of Physical Chemistry B, 2016, 120, 9223-9229.	2.6	18
143	Ferromagnetic Quantum Critical Point Avoided by the Appearance of Another Magnetic Phase in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>LaCrGe</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mr Pressure. Physical Review Letters, 2016, 117, 037207.	7.8	47
144	Correlation Matrix Renormalization Theory: Improving Accuracy with Two-Electron Density-Matrix Sum Rules. Journal of Chemical Theory and Computation, 2016, 12, 4806-4811.	5.3	14

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145	Studies on optical properties of Si220 nanoclusters via time-dependent density functional theory calculations. Chemical Research in Chinese Universities, 2016, 32, 1028-1033.	2.6	1
146	Crystal structure and magnetic properties of new Fe₃Co₃X₂(Xâ€‰â€‰=â€‰â€‰Ti, Nb) intermetallic compounds. Journal Physics D: Applied Physics, 2016, 49, 175002.	2.8	11
147	Gutzwiller renormalization group. Physical Review B, 2016, 93, .	3.2	4
148	Interplay between surface and surface resonance states on height selective stability of fcc Dy(111) film at nanoscale. Physical Chemistry Chemical Physics, 2016, 18, 31238-31243.	2.8	2
149	Metastable cobalt nitride structures with high magnetic anisotropy for rare-earth free magnets. Physical Chemistry Chemical Physics, 2016, 18, 31680-31690.	2.8	28
150	Cooling rate dependence of structural order in Al90Sm10 metallic glass. Journal of Applied Physics, 2016, 120, .	2.5	43
151	â€˜Crystal Genesâ€™ in Metallic Liquids and Glasses. Scientific Reports, 2016, 6, 23734.	3.3	52
152	Zero-Strain Na₂FeSiO₄ as Novel Cathode Material for Sodium-Ion Batteries. ACS Applied Materials & Interfaces, 2016, 8, 17233-17238.	8.0	101
153	Stabilities and defect-mediated lithium-ion conduction in a ground state cubic Li₃N structure. Physical Chemistry Chemical Physics, 2016, 18, 4185-4190.	2.8	5
154	Tight-binding calculation studies of vacancy and adatom defects in graphene. Journal of Physics Condensed Matter, 2016, 28, 115001.	1.8	17
155	Charge oscillations and interaction between potassium adatoms on graphene studied by first-principles calculations. Physical Review B, 2015, 91, .	3.2	9
156	Three-center tight-binding potential model for C and Si. Physical Review B, 2015, 92, .	3.2	17
157	Efficient and accurate treatment of electron correlations with Correlation Matrix Renormalization theory. Scientific Reports, 2015, 5, 13478.	3.3	11
158	Structures and magnetic properties of Co-Zr-B magnets studied by first-principles calculations. Journal of Applied Physics, 2015, 117, .	2.5	15
159	A computational study of diffusion in a glass-forming metallic liquid. Scientific Reports, 2015, 5, 10956.	3.3	11
160	Local structure order in Pd78Cu6Si16 liquid. Scientific Reports, 2015, 5, 8277.	3.3	26
161	Dynamics and Diffusion Mechanism of Low-Density Liquid Silicon. Journal of Physical Chemistry B, 2015, 119, 14945-14951.	2.6	2
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