Kai Ming Ho

List of Publications by Year
in descending order

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227	8,034	71004	66518
papers	citations	43 h-index	82 g-index

240	240	240	8493
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A three-dimensional photonic crystal operating at infrared wavelengths. Nature, 1998, 394, 251-253.	13.7	1,034
2	Structures of medium-sized silicon clusters. Nature, 1998, 392, 582-585.	13.7	622
3	Melting line of aluminum from simulations of coexisting phases. Physical Review B, 1994, 49, 3109-3115.	1.1	438
4	On-the-fly machine-learning for high-throughput experiments: search for rare-earth-free permanent magnets. Scientific Reports, 2014, 4, 6367.	1.6	212
5	Experimental and theoretical results for a twoâ€dimensional metal photonic bandâ€gap cavity. Applied Physics Letters, 1994, 65, 645-647.	1.5	171
6	Bonding and charge transfer by metal adatom adsorption on graphene. Physical Review B, 2011, 83, .	1.1	167
7	The geometry of small fullerene cages: C20 to C70. Journal of Chemical Physics, 1992, 97, 5007-5011.	1.2	145
8	Metals on Graphene: Interactions, Growth Morphology, and Thermal Stability. Crystals, 2013, 3, 79-111.	1.0	135
9	Modeling ionic mobilities by scattering on electronic density isosurfaces: Application to silicon cluster anions. Journal of Chemical Physics, 2000, 112, 4517-4526.	1.2	131
10	Broadband optical absorption by tunable Mie resonances in silicon nanocone arrays. Scientific Reports, 2015, 5, 7810.	1.6	126
11	Structures of Germanium Clusters: Where the Growth Patterns of Silicon and Germanium Clusters Diverge. Physical Review Letters, 1999, 83, 2167-2170.	2.9	123
12	Atomistic cluster alignment method for local order mining in liquids and glasses. Physical Review B, 2010, 82, .	1.1	120
13	An adaptive genetic algorithm for crystal structure prediction. Journal of Physics Condensed Matter, 2014, 26, 035402.	0.7	120
14	The geometry of large fullerene cages: C72 to C102. Journal of Chemical Physics, 1993, 98, 3095-3102.	1.2	105
15	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
16	Zero-Strain Na₂FeSiO₄ as Novel Cathode Material for Sodium-Ion Batteries. ACS Applied Materials & Interfaces, 2016, 8, 17233-17238.	4.0	101
17	Prediction of a {1122} hcp stacking fault using a modified generalized stacking-fault calculation. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1997, 76, 1065-1077.	0.8	100
18	Exploring the Structural Complexity of Intermetallic Compounds by an Adaptive Genetic Algorithm. Physical Review Letters, 2014, 112, 045502.	2.9	97

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19	Structures and Fragmentations of Small Silicon Oxide Clusters by ab Initio Calculations. Journal of Physical Chemistry A, 2003, 107, 6936-6943.	1.1	94
20	Spectroscopic Evidence for the Tricapped Trigonal Prism Structure of Semiconductor Clusters. Physical Review Letters, 2000, 85, 1666-1669.	2.9	91
21	Quasiatomic orbitals forab initiotight-binding analysis. Physical Review B, 2008, 78, .	1.1	90
22	Vacancy defects and the formation of local haeckelite structures in graphene from tight-binding molecular dynamics. Physical Review B, 2006, 74, .	1.1	81
23	Infrared filters using metallic photonic band gap structures on flexible substrates. Applied Physics Letters, 1997, 71, 2412-2414.	1.5	77
24	Lattice symmetry applied in transfer-matrix methods for photonic crystals. Journal of Applied Physics, 2003, 94, 811-821.	1.1	77
25	Search for the groundâ€state structure of C84. Journal of Chemical Physics, 1992, 96, 7183-7185.	1.2	72
26	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
27	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
28	Phase Diagram and Electronic Structure of Praseodymium and Plutonium. Physical Review X, 2015, 5, .	2.8	67
29	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
30	Representation of electronic structures in crystals in terms of highly localized quasiatomic minimal basis orbitals. Physical Review B, 2004, 70, .	1.1	63
31	Adaptive Variational Quantum Dynamics Simulations. PRX Quantum, 2021, 2, .	3.5	57
32	Dipole antennas on photonic band-gap crystals?Experiment and simulation. Microwave and Optical Technology Letters, 1997, 15, 153-158.	0.9	56
33	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
34	Reconstruction and evaporation at graphene nanoribbon edges. Physical Review B, 2010, 81, .	1.1	55
35	â€˜Crystal Genesâ€™ in Metallic Liquids and Glasses. Scientific Reports, 2016, 6, 23734.	1.6	52
36	Effects of sub-Tg annealing on Cu64.5Zr35.5 glasses: A molecular dynamics study. Applied Physics Letters, 2014, 104, .	1.5	51

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37	Melting of small Sn clusters byab initiomolecular dynamics simulations. Physical Review B, 2004, 69, .	1.1	50
38	Evaluation of Ionic Mobilities by Coupling the Scattering on Atoms and on Electron Density. Journal of Physical Chemistry A, 2000, 104, 6152-6157.	1.1	49
39	Structure and dynamics of liquid Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><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" display="inline"><mml:mrow><mml:msub><mml:mrow />	1.1	48
40	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:mrow> Pressure. Physical Review Letters, 2016, 117, 037207.	2.9	47
41	Identification of post-pyrite phase transitions in SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>by a genetic algorithm. Physical Review B, 2011, 83, .	1.1	46
42	Overcoming the Time Limitation in Molecular Dynamics Simulation of Crystal Nucleation: A Persistent-Embryo Approach. Physical Review Letters, 2018, 120, 085703.	2.9	46
43	Short- and medium-range order in a<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:mrow><mml:mn>7</mml:mn></mml:mrow> Experimental and simulation studies. Physical Review B, 2008, 78, .	1.1	43
44	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
45	Impedance of photonic crystals and photonic crystal waveguides. Applied Physics Letters, 2004, 84, 1254-1256.	1.5	43
46	Cooling rate dependence of structural order in Al90Sm10 metallic glass. Journal of Applied Physics, 2016, 120, .	1.1	43
47	Efficient Step-Merged Quantum Imaginary Time Evolution Algorithm for Quantum Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 6256-6266.	2.3	42
48	Highly localized quasiatomic minimal basis orbitals for Mo fromab initiocalculations. Physical Review B, 2007, 76, .	1.1	41
49	Interface Structure Prediction from First-Principles. Journal of Physical Chemistry C, 2014, 118, 9524-9530.	1.5	39
50	Development of a deep machine learning interatomic potential for metalloid-containing Pd-Si compounds. Physical Review B, 2019, 100, .	1.1	39
51	Short- and medium-range order in amorphous<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:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub> alloy. Physical Review B, 2010, 81, .	1.1	38
52	Growth morphology and thermal stability of metal islands on graphene. Physical Review B, 2012, 86, .	1.1	38
53	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
54	Waveguide bends in three-dimensional layer-by-layer photonic bandgap materials. Microwave and Optical Technology Letters, 1999, 23, 56-59.	0.9	36

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55	Predicting Complex Relaxation Processes in Metallic Glass. Physical Review Letters, 2019, 123, 105701.	2.9	36
56	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
57	High Efficiency GaN Light-Emitting Diodes With Two Dimensional Photonic Crystal Structures of Deep-Hole Square Lattices. IEEE Journal of Quantum Electronics, 2010, 46, 116-120.	1.0	34
58	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
59	Formation of carbon nanotube semiconductor-metal intramolecular junctions by self-assembly of vacancy defects. Physical Review B, 2007, 76, .	1.1	32
60	Design of midinfrared photodetectors enhanced by resonant cavities with subwavelength metallic gratings. Applied Physics Letters, 2008, 93, .	1.5	32
61	Adaptive Variational Quantum Imaginary Time Evolution Approach for Ground State Preparation. Advanced Quantum Technologies, 2021, 4, 2100114.	1.8	32
62	Formation and development of dislocation in graphene. Applied Physics Letters, 2013, 102, .	1.5	31
63	Waveguide networks in three-dimensional layer-by-layer photonic crystals. Applied Physics Letters, 2004, 84, 4605-4607.	1.5	30
64	Effects of Nanometer-Scale Photonic Crystal Structures on the Light Extraction From GaN Light-Emitting Diodes. IEEE Journal of Quantum Electronics, 2010, 46, 1375-1380.	1.0	30
65	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></mml:mrow></mml:math> . Physical Review B, 2011, 84, .	1.1	29
66	Unique Dynamic Appearance of a Ge-Si Ad-dimer on Si(001). Physical Review Letters, 2000, 85, 5603-5606.	2.9	28
67	Structures and magnetic properties of Fe clusters on graphene. Physical Review B, 2014, 90, .	1.1	28
68	Metastable cobalt nitride structures with high magnetic anisotropy for rare-earth free magnets. Physical Chemistry Chemical Physics, 2016, 18, 31680-31690.	1.3	28
69	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
70	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
71	Topochemical Deintercalation of Li from Layered LiNiB: toward 2D MBene. Journal of the American Chemical Society, 2021, 143, 4213-4223.	6.6	28
72	Transferability of the Slater-Koster tight-binding scheme from an environment-dependent minimal-basis perspective. Physical Review B, 2005, 72, .	1.1	27

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73	Exploration of tetrahedral structures in silicate cathodes using a motif-network scheme. Scientific Reports, 2015, 5, 15555.	1.6	27
74	Feâ€“Si networks in Na₂FeSiO₄ cathode materials. Physical Chemistry Chemical Physics, 2016, 18, 23916-23922.	1.3	27
75	Local structure order in Pd78Cu6Si16 liquid. Scientific Reports, 2015, 5, 8277.	1.6	26
76	Structures and energies of compression twin boundaries inhcpTi and Zr. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1995, 72, 751-763.	0.8	25
77	Light coupling with multimode photonic crystal waveguides. Applied Physics Letters, 2004, 84, 4699-4701.	1.5	25
78	Improved surface wettability of polyurethane films by ultraviolet ozone treatment. Journal of Applied Polymer Science, 2010, 118, 3024-3033.	1.3	25
79	Structural characterization of thin film photonic crystals. Physical Review B, 2001, 63, .	1.1	24
80	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
81	Computationally Driven Discovery of a Family of Layered LiNiB Polymorphs. Angewandte Chemie - International Edition, 2019, 58, 15855-15862.	7.2	24
82	Fe-Fe adatom interaction and growth morphology on graphene. Physical Review B, 2011, 84, .	1.1	23
83	Nature of the Insulating Ground State of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>5</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>Postperovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>CaIrO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Letters, 2015, 115, 096401.	2.9	22
84	A first-principles study of Group IV dimer chains on Si(100). Physical Review B, 2005, 72, .	1.1	21
85	Gutzwiller hybrid quantum-classical computing approach for correlated materials. Physical Review Research, 2021, 3, .	1.3	21
86	Visible Frequency Thin Film Photonic Crystals from Colloidal Systems of Nanocrystalline Titania and Polystyrene Microspheres. Journal of the American Ceramic Society, 2002, 85, 1383-1386.	1.9	20
87	Honeycomb chain structure of theAuâ•Si(111)â^'(5Ã—2)surface reconstruction: A first-principles study. Physical Review B, 2008, 77, .	1.1	20
88	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
89	Interplay of spin-orbit and entropic effects in cerium. Physical Review B, 2014, 90, .	1.1	20
90	Local structure origin of ultrafast crystallization driven by high-fidelity octahedral clusters in amorphous Sc0.2Sb2Te3. Applied Physics Letters, 2019, 114, .	1.5	20

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91	Model reconstructions for the Si(337) orientation. Journal of Applied Physics, 2005, 98, 073507.	1.1	19
92	Tailored Plasmons in Pentacene/Graphene Heterostructures with Interlayer Electron Transfer. Nano Letters, 2019, 19, 6058-6064.	4.5	19
93	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
94	Tight-Binding Molecular Dynamics Studies of Covalent Systems. Advances in Chemical Physics, 2007, , 651-702.	0.3	18
95	Effects of Oxygen Impurities on Glass-Formation Ability in Zr₂Cu Alloy. Journal of Physical Chemistry B, 2016, 120, 9223-9229.	1.2	18
96	Material simulations with tight-binding molecular dynamics. Journal of Phase Equilibria and Diffusion, 1997, 18, 516-529.	0.3	17
97	Double icosahedronâ€based motif of Ni_n (n = 20â”30). International Journal of Quantum Chemistry, 2012, 112, 1717-1724.	1.0	17
98	Three-center tight-binding potential model for C and Si. Physical Review B, 2015, 92, .	1.1	17
99	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
100	A first-principles study of compression twins in h.c.p. zirconium. Philosophical Magazine Letters, 1994, 69, 189-195.	0.5	16
101	Fluctuation between icosahedral and body-centered-cube short-range orders in undercooled Zr liquid. Journal of Applied Physics, 2011, 110, .	1.1	16
102	Topological states in A15 superconductors. Physical Review B, 2019, 99, .	1.1	16
103	The role of pentagonâ€“heptagon pair defect in carbon nanotube: The center of vacancy reconstruction. Applied Physics Letters, 2010, 97, 093106.	1.5	15
104	Nonclassical â€œExplosiveâ€•Nucleation in Pb/Si(111) at Low Temperatures. Physical Review Letters, 2014, 113, 236101.	2.9	15
105	Unraveling the structural and bonding nature of antimony sesquichalcogenide glass for electronic and photonic applications. Journal of Materials Chemistry C, 0, , .	2.7	15
106	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
107	Melting of carbon cages. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 285-287.	1.0	14
108	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

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109	Structures and stability of metal-doped GenM (n = 9, 10) clusters. AIP Advances, 2015, 5, .	0.6	14
110	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
111	Polyamorphism in K₂Sb₈Se₁₃ for multi-level phase-change memory. Journal of Materials Chemistry C, 2020, 8, 6364-6369.	2.7	14
112	Structural hierarchy as a key to complex phase selection in Al-Sm. Physical Review Materials, 2017, 1, .	0.9	14
113	Two-step nucleation of the Earthâ€™s inner core. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	14
114	Medium-range icosahedral order in quasicrystal-forming Zr2Pd binary metallic glass. Applied Physics Letters, 2011, 98, .	1.5	13
115	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
116	Synergistic computational and experimental discovery of novel magnetic materials. Molecular Systems Design and Engineering, 2020, 5, 1098-1117.	1.7	13
117	Competition between area and height evolution of Pb islands on a Si(111) surface. Physical Review B, 2009, 79, .	1.1	12
118	Structural features of chalcogenide glass SiTe: An ovonic threshold switching material. APL Materials, 2021, 9, .	2.2	12
119	Achieving a photonic band edge near visible wavelengths by metallic coatings. Journal of Applied Physics, 2006, 99, 083104.	1.1	11
120	Analysis of photon recycling using metallic photonic crystal. Journal of Applied Physics, 2007, 102, 063107.	1.1	11
121	Efficient and accurate treatment of electron correlations with Correlation Matrix Renormalization theory. Scientific Reports, 2015, 5, 13478.	1.6	11
122	A computational study of diffusion in a glass-forming metallic liquid. Scientific Reports, 2015, 5, 10956.	1.6	11
123	Manipulation of electronic property of epitaxial graphene on SiC substrate by Pb intercalation. Physical Review B, 2021, 103, .	1.1	11
124	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	0.9	11
125	Structures ofSi7H2m(m=1â€“7)clusters by global optimization. Physical Review B, 2006, 74, .	1.1	10
126	Theoretical Prediction of Si₂â€“Si₃₃ Absorption Spectra. Journal of Physical Chemistry A, 2017, 121, 6388-6397.	1.1	10

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127	Effects of dopants on the glass forming ability in Al-based metallic alloy. Physical Review Materials, 2019, 3, .	0.9	10
128	Integrated horns for improved side coupling into in-plane three-dimensional photonic crystal waveguides. Applied Physics Letters, 2004, 85, 707-709.	1.5	9
129	Tight-binding Hamiltonian from first-principles calculations. Scientific Modeling and Simulation SMNS, 2008, 15, 81-95.	0.8	9
130	Global Optimization of 2-Dimensional Nanoscale Structures: A Brief Review. Materials and Manufacturing Processes, 2009, 24, 109-118.	2.7	9
131	Charge oscillations and interaction between potassium adatoms on graphene studied by first-principles calculations. Physical Review B, 2015, 91, .	1.1	9
132	Electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ce</mml:mi><mml:mn>2</mml:mn></mml: A two-dimensional heavy-fermion system studied by angle-resolved photoemission spectroscopy. Physical Review B, 2015, 91, .	1.1	9
133	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.	5.2	9
134	Theoretical search for possible Au-Si crystal structures using a genetic algorithm. Physical Review B, 2017, 95, .	1.1	9
135	Phase Diagram and Structure Map of Binary Nanoparticle Superlattices from a Lennard-Jones Model. ACS Nano, 2020, 14, 6795-6802.	7.3	9
136	Molecular dynamics simulation of metallic Alâ€“Ce liquids using a neural network machine learning interatomic potential. Journal of Chemical Physics, 2021, 155, 194503.	1.2	9
137	Atomic and electronic structures of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Ag</mml:mtext><mml:mo>/</mml:mo><mml:mtext>Si</mml:mtext><mml: A first-principles study. Physical Review B, 2008, 78, .	1.1	8
138	Thermodynamic limits of crystallization and the prediction of glass formation tendency. Physical Review B, 2010, 81, .	1.1	8
139	Quantum confinement induced oscillatory electric field on a stepped Pb(111) film and its influence on surface reactivity. Physical Review B, 2014, 89, .	1.1	8
140	Structure and magnetism of new rare-earth-free intermetallic compounds: Fe3+xCo3â^'xTi2 (0 â‰¤ x â‰¤ 3). APL Materials, 2016, 4, .	2.2	8
141	Structures, phase transitions, and magnetic properties of Co3Si from first-principles calculations. Physical Review B, 2017, 96, .	1.1	8
142	Spatial decomposition of magnetic anisotropy in magnets: Application to doped Fe16N2. Physical Review B, 2020, 102, .	1.1	8
143	Stabilizing the crystal structures of NaFePO₄ with Li substitutions. Physical Chemistry Chemical Physics, 2020, 22, 13975-13980.	1.3	8
144	Theoretical search for possible Liâ€“Niâ€“B crystal structures using an adaptive genetic algorithm. Journal of Applied Physics, 2020, 127, .	1.1	8

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145	Electronic Structure of Double-Layer Epitaxial Graphene on SiC(0001) Modified by Gd Intercalation. Journal of Physical Chemistry C, 2020, 124, 28132-28138.	1.5	8
146	Deep machine learning potential for atomistic simulation of Fe-Si-O systems under Earth's outer core conditions. Physical Review Materials, 2022, 6, .	0.9	8
147	Tight-binding molecular dynamics for materials simulations. Journal of Computer-Aided Materials Design, 1996, 3, 139-148.	0.7	7
148	Cluster expansion modeling and Monte Carlo simulation of alnico 5â€“7 permanent magnets. Journal of Applied Physics, 2015, 117, .	1.1	7
149	Metal intercalation-induced selective adatom mass transport on graphene. Nano Research, 2016, 9, 1434-1441.	5.8	7
150	Cluster-Expansion Model for Complex Quinary Alloys: Application to Alnico Permanent Magnets. Physical Review Applied, 2017, 8, .	1.5	7
151	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.	1.5	7
152	Lithium nickel borides: evolution of [NiB] layers driven by Li pressure. Inorganic Chemistry Frontiers, 2021, 8, 1675-1685.	3.0	7
153	Characterizations of electronic and optical properties of Sb-based phase-change material stabilized by alloying Cr. Applied Physics Letters, 2021, 118, .	1.5	7
154	Nonequilibrium phonon tuning and mapping in few-layer graphene with infrared nanoscopy. Physical Review B, 2021, 103, .	1.1	7
155	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:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> clusters. Physical Review Materials, 2018, 2, .	0.9	7
156	Environment-Dependent Tight-Binding Potential Model. Materials Research Society Symposia Proceedings, 1997, 491, 211.	0.1	6
157	Stochastic coarsening model for Pb islands on a Si(111) surface. Physical Review B, 2010, 82, .	1.1	6
158	Atomic Structure and Magnetic Properties of HfCo$_{7}$ Alloy. IEEE Transactions on Magnetics, 2013, 49, 3281-3283.	1.2	6
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