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	Neural network potential for Zrâ€“Rh system by machine learning. Journal of Physics Condensed Matter, 2022, 34, 075402.	0.7	6
2	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
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, .	0.9	3
4	Straintronic Effect on Phonon-Mediated Superconductivity of Nb₂CT₂ (T = O,) Tj ETQq0 0 0 rgBT /Overlock 10	1.5	5
5	Reversible motions and disordered structure of soft particles in amorphous solids. Physical Review B, 2022, 105, .	1.1	0
6	The Gutzwiller conjugate gradient minimization method for correlated electron systems. Journal of Physics Condensed Matter, 2022, 34, 243001.	0.7	4
7	Structure and motifs of iron oxides from 1 to 3 TPa. Physical Review Materials, 2022, 6, .	0.9	1
8	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
9	Ground state wave functions for single-band Hubbard models from the Gutzwiller conjugate gradient minimisation theory. Molecular Physics, 2021, 119, e1797917.	0.8	5
10	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.	0.8	3
11	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
12	Localized electronic and vibrational states in amorphous diamond. Physical Chemistry Chemical Physics, 2021, 23, 4835-4840.	1.3	2
13	Lithium nickel borides: evolution of [NiB] layers driven by Li pressure. Inorganic Chemistry Frontiers, 2021, 8, 1675-1685.	3.0	7
14	Characterizations of electronic and optical properties of Sb-based phase-change material stabilized by alloying Cr. Applied Physics Letters, 2021, 118, .	1.5	7
15	Gutzwiller hybrid quantum-classical computing approach for correlated materials. Physical Review Research, 2021, 3, .	1.3	21
16	Manipulation of electronic property of epitaxial graphene on SiC substrate by Pb intercalation. Physical Review B, 2021, 103, .	1.1	11
17	Evidence for a large Rashba splitting in PtPb4 from angle-resolved photoemission spectroscopy. Physical Review B, 2021, 103, .	1.1	3
18	Topochemical Deintercalation of Li from Layered LiNiB: toward 2D MBene. Journal of the American Chemical Society, 2021, 143, 4213-4223.	6.6	28

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19	Unveiling the mechanism of phase and morphology selections during the devitrification of Al-Sm amorphous ribbon. Physical Review Materials, 2021, 5, .	0.9	3
20	Nonequilibrium phonon tuning and mapping in few-layer graphene with infrared nanoscopy. Physical Review B, 2021, 103, .	1.1	7
21	Ternary Zinc Antimonides Unlocked Using Hydride Synthesis. Inorganic Chemistry, 2021, 60, 10686-10697.	1.9	6
22	Adaptive Variational Quantum Dynamics Simulations. PRX Quantum, 2021, 2, .	3.5	57
23	Role of Coulomb interaction in the phase formation of fcc Ce: Correlation matrix renormalization theory. Physical Review B, 2021, 104, .	1.1	6
24	Structural features of chalcogenide glass SiTe: An ovonic threshold switching material. APL Materials, 2021, 9, .	2.2	12
25	How to Look for Compounds: Predictive Screening and inâ€…situ Studies in Naâ^'Znâ^'Bi System. Chemistry - A European Journal, 2021, 27, 15954-15966.	1.7	4
26	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
27	Correlation matrix renormalization theory in multi-band lattice systems. Journal of Physics Condensed Matter, 2021, 33, 095902.	0.7	3
28	Adaptive Variational Quantum Imaginary Time Evolution Approach for Ground State Preparation. Advanced Quantum Technologies, 2021, 4, 2100114.	1.8	32
29	Unconventional iron-magnesium compounds at terapascal pressures. Physical Review B, 2021, 104, .	1.1	3
30	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
31	Pressure-induced superconductivity in the hydrogen-rich pseudobinary CaBâ^'Hn compounds. Physical Review B, 2021, 104, .	1.1	5
32	Lithium Diffusion in Silicon Encapsulated with Graphene. Nanomaterials, 2021, 11, 3397.	1.9	3
33	Defect Interaction and Deformation in Graphene. Journal of Physical Chemistry C, 2020, 124, 2370-2378.	1.5	6
34	Efficient Step-Merged Quantum Imaginary Time Evolution Algorithm for Quantum Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 6256-6266.	2.3	42
35	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
36	Spatial decomposition of magnetic anisotropy in magnets: Application to doped Fe16N2. Physical Review B, 2020, 102, .	1.1	8

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37	Phase Diagram and Structure Map of Binary Nanoparticle Superlattices from a Lennard-Jones Model. ACS Nano, 2020, 14, 6795-6802.	7.3	9
38	Stabilizing the crystal structures of NaFePO₄ with Li substitutions. Physical Chemistry Chemical Physics, 2020, 22, 13975-13980.	1.3	8
39	Synergistic computational and experimental discovery of novel magnetic materials. Molecular Systems Design and Engineering, 2020, 5, 1098-1117.	1.7	13
40	Unveiling the medium-range order in glass models and its role in glass formation. Physical Review B, 2020, 101, .	1.1	5
41	Characterization of three phases of liquid carbon by tight-binding molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 14630-14636.	1.3	4
42	Theoretical search for possible Liâ€“Niâ€“B crystal structures using an adaptive genetic algorithm. Journal of Applied Physics, 2020, 127, .	1.1	8
43	First-principles calculation of excited states of diatomic molecules: a benchmark for the Gutzwiller conjugate gradient minimisation method. Molecular Physics, 2020, 118, .	0.8	6
44	Polyamorphism in K₂Sb₈Se₁₃ for multi-level phase-change memory. Journal of Materials Chemistry C, 2020, 8, 6364-6369.	2.7	14
45	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
46	Cryogenic spatialâ€“temporal imaging of surface photocarrier dynamics in MAPbI3 films at the single grain level. AIP Advances, 2020, 10, .	0.6	2
47	Discovering rare-earth-free magnetic materials through the development of a database. Physical Review Materials, 2020, 4, .	0.9	11
48	HOT Graphene and HOT Graphene Nanotubes: New Low Dimensional Semimetals and Semiconductors. Nanoscale Research Letters, 2020, 15, 56.	3.1	4
49	Tailored Plasmons in Pentacene/Graphene Heterostructures with Interlayer Electron Transfer. Nano Letters, 2019, 19, 6058-6064.	4.5	19
50	Computationally Driven Discovery of a Family of Layered LiNiB Polymorphs. Angewandte Chemie - International Edition, 2019, 58, 15855-15862.	7.2	24
51	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
52	Theoretical prediction of a highly responsive material: Spin fluctuations and superconductivity in FeNiB2 system. Applied Physics Letters, 2019, 115, 182601.	1.5	4
53	Development of a deep machine learning interatomic potential for metalloid-containing Pd-Si compounds. Physical Review B, 2019, 100, .	1.1	39
54	Predicting Complex Relaxation Processes in Metallic Glass. Physical Review Letters, 2019, 123, 105701.	2.9	36

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55	Strong optical absorption of a metallic film to induce a lensing effect in the visible region. Scientific Reports, 2019, 9, 12434.	1.6	1
56	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
57	Observation of Î·-Al41Sm5 reveals motif-aware structural evolution in Al-Sm alloys. Scientific Reports, 2019, 9, 6692.	1.6	4
58	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, .	1.1	4
59	Topological states in A15 superconductors. Physical Review B, 2019, 99, .	1.1	16
60	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.	1.5	6
61	Local structure origin of ultrafast crystallization driven by high-fidelity octahedral clusters in amorphous Sc0.2Sb2Te3. Applied Physics Letters, 2019, 114, .	1.5	20
62	Effects of dopants on the glass forming ability in Al-based metallic alloy. Physical Review Materials, 2019, 3, .	0.9	10
63	Microstructure evolution during near- Tg annealing and its effect on shear banding in model alloys. Physical Review Materials, 2019, 3, .	0.9	3
64	Overcoming the Time Limitation in Molecular Dynamics Simulation of Crystal Nucleation: A Persistent-Embryo Approach. Physical Review Letters, 2018, 120, 085703.	2.9	46
65	Ternary Bismuthide SrPtBi₂: Computation and Experiment in Synergism to Explore Solid-State Materials. Journal of Physical Chemistry C, 2018, 122, 5057-5063.	1.5	4
66	A comparative study of Sm networks in Al-10 at.%Sm glass and associated crystalline phases. Philosophical Magazine Letters, 2018, 98, 27-37.	0.5	2
67	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
68	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, .	1.1	6
69	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
70	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
71	Structures and magnetic properties of iron silicide from adaptive genetic algorithm and first-principles calculations. Journal of Applied Physics, 2018, 124, .	1.1	6
72	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

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73	High 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></mml:math> 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></mml:math> compounds from first-principles real-space pseudopotentials calculations. Physical Review Materials, 2018, 2, .	0.9	4
74	Hybrid siliconâ€“carbon nanostructures for broadband optical absorption. RSC Advances, 2017, 7, 8070-8076.	1.7	5
75	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
76	Growth and characterization of BaZnGa. Philosophical Magazine, 2017, 97, 3317-3324.	0.7	0
77	Structures, phase transitions, and magnetic properties of Co3Si from first-principles calculations. Physical Review B, 2017, 96, .	1.1	8
78	Fe-Cluster Compounds of Chalcogenides: Candidates for Rare-Earth-Free Permanent Magnet and Magnetic Nodal-Line Topological Material. Inorganic Chemistry, 2017, 56, 14577-14583.	1.9	4
79	Cluster-Expansion Model for Complex Quinary Alloys: Application to Alnico Permanent Magnets. Physical Review Applied, 2017, 8, .	1.5	7
80	Theoretical Prediction of Si₂â€“Si₃₃ Absorption Spectra. Journal of Physical Chemistry A, 2017, 121, 6388-6397.	1.1	10
81	Theoretical search for possible Au-Si crystal structures using a genetic algorithm. Physical Review B, 2017, 95, .	1.1	9
82	Structural hierarchy as a key to complex phase selection in Al-Sm. Physical Review Materials, 2017, 1, .	0.9	14
83	Simulations of enhance broadband optical absorption by tuning mie resonance in silicon nanocone arrays. , 2016, , .		0
84	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
85	Metal intercalation-induced selective adatom mass transport on graphene. Nano Research, 2016, 9, 1434-1441.	5.8	7
86	Feâ€“Si networks in Na₂FeSiO₄ cathode materials. Physical Chemistry Chemical Physics, 2016, 18, 23916-23922.	1.3	27
87	Effects of Oxygen Impurities on Glass-Formation Ability in Zr₂Cu Alloy. Journal of Physical Chemistry B, 2016, 120, 9223-9229.	1.2	18
88	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></mml:msub></mml:mrow></mml:math> Pressure. Physical Review Letters, 2016, 117, 037207.	2.9	47
89	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
90	Gutzwiller renormalization group. Physical Review B, 2016, 93, .	1.1	4

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91	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.	1.3	2
92	Metastable cobalt nitride structures with high magnetic anisotropy for rare-earth free magnets. Physical Chemistry Chemical Physics, 2016, 18, 31680-31690.	1.3	28
93	Cooling rate dependence of structural order in Al90Sm10 metallic glass. Journal of Applied Physics, 2016, 120, .	1.1	43
94	â€˜Crystal Genesâ€™ in Metallic Liquids and Glasses. Scientific Reports, 2016, 6, 23734.	1.6	52
95	Zero-Strain Na₂FeSiO₄ as Novel Cathode Material for Sodium-Ion Batteries. ACS Applied Materials & Interfaces, 2016, 8, 17233-17238.	4.0	101
96	Stabilities and defect-mediated lithium-ion conduction in a ground state cubic Li₃N structure. Physical Chemistry Chemical Physics, 2016, 18, 4185-4190.	1.3	5
97	Charge oscillations and interaction between potassium adatoms on graphene studied by first-principles calculations. Physical Review B, 2015, 91, .	1.1	9
98	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
99	Three-center tight-binding potential model for C and Si. Physical Review B, 2015, 92, .	1.1	17
100	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></ Physical Review Letters, 2015, 115, 096401.	2.9	22
101	Efficient and accurate treatment of electron correlations with Correlation Matrix Renormalization theory. Scientific Reports, 2015, 5, 13478.	1.6	11
102	Exploration of tetrahedral structures in silicate cathodes using a motif-network scheme. Scientific Reports, 2015, 5, 15555.	1.6	27
103	A computational study of diffusion in a glass-forming metallic liquid. Scientific Reports, 2015, 5, 10956.	1.6	11
104	Local structure order in Pd78Cu6Si16 liquid. Scientific Reports, 2015, 5, 8277.	1.6	26
105	Dynamics and Diffusion Mechanism of Low-Density Liquid Silicon. Journal of Physical Chemistry B, 2015, 119, 14945-14951.	1.2	2
106	Broadband optical absorption by tunable Mie resonances in silicon nanocone arrays. Scientific Reports, 2015, 5, 7810.	1.6	126
107	Phase Diagram and Electronic Structure of Praseodymium and Plutonium. Physical Review X, 2015, 5, .	2.8	67
108	Cluster expansion modeling and Monte Carlo simulation of alnico 5â€“7 permanent magnets. Journal of Applied Physics, 2015, 117, .	1.1	7

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109	Structures and stability of metal-doped GenM (n = 9, 10) clusters. AIP Advances, 2015, 5, .	0.6	14
110	Nonclassical â€œExplosiveâ€•Nucleation in Pb/Si(111) at Low Temperatures. Physical Review Letters, 2014, 113, 236101.	2.9	15
111	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
112	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
113	Structure of Cu64.5Zr35.5 metallic glass by reverse Monte Carlo simulations. Journal of Applied Physics, 2014, 115, 053522.	1.1	6
114	Structures and magnetic properties of Fe clusters on graphene. Physical Review B, 2014, 90, .	1.1	28
115	Interplay of spin-orbit and entropic effects in cerium. Physical Review B, 2014, 90, .	1.1	20
116	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
117	Effects of sub-Tg annealing on Cu64.5Zr35.5 glasses: A molecular dynamics study. Applied Physics Letters, 2014, 104, .	1.5	51
118	An adaptive genetic algorithm for crystal structure prediction. Journal of Physics Condensed Matter, 2014, 26, 035402.	0.7	120
119	New Be-intercalated hexagonal boron layer structure of BeB2. RSC Advances, 2014, 4, 15061-15065.	1.7	5
120	Ultrafast Bulk Diffusion of AlH_x in High-Entropy Dehydrogenation Intermediates of NaAlH₄. Journal of Physical Chemistry C, 2014, 118, 18356-18361.	1.5	3
121	Interface Structure Prediction from First-Principles. Journal of Physical Chemistry C, 2014, 118, 9524-9530.	1.5	39
122	Exploring the Structural Complexity of Intermetallic Compounds by an Adaptive Genetic Algorithm. Physical Review Letters, 2014, 112, 045502.	2.9	97
123	On-the-fly machine-learning for high-throughput experiments: search for rare-earth-free permanent magnets. Scientific Reports, 2014, 4, 6367.	1.6	212
124	Atomic Structure and Magnetic Properties of HfCo$_{7}$ Alloy. IEEE Transactions on Magnetics, 2013, 49, 3281-3283.	1.2	6
125	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
126	Formation and development of dislocation in graphene. Applied Physics Letters, 2013, 102, .	1.5	31

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127	Influence of oriented topological defects on the mechanical properties of carbon nanotube heterojunctions. Journal of Applied Physics, 2013, 114, 144306.	1.1	2
128	The Genetic Algorithm in Real-Space Representation. , 2013, , 11-35.		0
129	Metals on Graphene: Interactions, Growth Morphology, and Thermal Stability. Crystals, 2013, 3, 79-111.	1.0	135
130	Growth morphology and thermal stability of metal islands on graphene. Physical Review B, 2012, 86, .	1.1	38
131	Double icosahedronâ€based motif of Ni_n (n = 20â^'30). International Journal of Quantum Chemistry, 2012, 112, 1717-1724.	1.0	17
132	The benchmark of Gutzwiller density functional theory in hydrogen systems. International Journal of Quantum Chemistry, 2012, 112, 240-246.	1.0	5
133	The benchmark of gutzwiller density functional theory in hydrogen systems. International Journal of Quantum Chemistry, 2012, 112, 2766-2766.	1.0	0
134	Fluctuation between icosahedral and body-centered-cube short-range orders in undercooled Zr liquid. Journal of Applied Physics, 2011, 110, .	1.1	16
135	Structure and dynamics of liquid N<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 /><mml:mrow><mml:mn>64</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>byab initi	1.1	48
136	Fe-Fe adatom interaction and growth morphology on graphene. Physical Review B, 2011, 84, .	1.1	23
137	Bonding and charge transfer by metal adatom adsorption on graphene. Physical Review B, 2011, 83, .	1.1	167
138	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
139	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
140	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
141	Structural stability of Cu₈₀Si₂₀ 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:math>initio molecular dynamics simulation. Physical Review B, 2011, 84, .	1.1	29
142	Medium-range icosahedral order in quasicrystal-forming Zr2Pd binary metallic glass. Applied Physics Letters, 2011, 98, .	1.5	13
143	Atomistic cluster alignment method for local order mining in liquids and glasses. Physical Review B, 2010, 82, .	1.1	120
144	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

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145	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
146	Improved surface wettability of polyurethane films by ultraviolet ozone treatment. Journal of Applied Polymer Science, 2010, 118, 3024-3033.	1.3	25
147	The role of pentagonâ€“heptagon pair defect in carbon nanotube: The center of vacancy reconstruction. Applied Physics Letters, 2010, 97, 093106.	1.5	15
148	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
149	Semicrystalline woodpile photonic crystals without complicated alignment via soft lithography. Applied Physics Letters, 2010, 96, .	1.5	5
150	Reconstruction and evaporation at graphene nanoribbon edges. Physical Review B, 2010, 81, .	1.1	55
151	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:mn>2</mml:mn></mml:msub alloy. Physical Review B, 2010, 81, .	1.1	38
152	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
153	Thermodynamic limits of crystallization and the prediction of glass formation tendency. Physical Review B, 2010, 81, .	1.1	8
154	Stochastic coarsening model for Pb islands on a Si(111) surface. Physical Review B, 2010, 82, .	1.1	6
155	Competition between area and height evolution of Pb islands on a Si(111) surface. Physical Review B, 2009, 79, .	1.1	12
156	Interfacial disorder and optoelectronic properties of diamond nanocrystals. Physical Review B, 2009, 80, .	1.1	4
157	Effects of defect permittivity on resonant frequency and mode shape in the three-dimensional woodpile photonic crystal. Journal of Applied Physics, 2009, 105, 103109.	1.1	5
158	Global Optimization of 2-Dimensional Nanoscale Structures: A Brief Review. Materials and Manufacturing Processes, 2009, 24, 109-118.	2.7	9
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