Ping Peng

List of Publications by Year
in descending order

203 papers	4,195 citations	117625 34 h-index	175258 52 g-index
203 all docs	203 docs citations	203 times ranked	4504 citing authors

#	Article	IF	Citations
1	Mechanical properties, thermophysical properties and electronic structure of Yb3+ or Ce4+-doped La2Zr2O7-based TBCs. Journal of Rare Earths, 2023, 41, 588-598.	4.8	2
2	Competition between TCP and crystalline clusters during phase transition of rapidly super-cooled aluminum. Journal of Non-Crystalline Solids, 2022, 576, 121271.	3.1	8
3	First-principles investigations of the fracture toughness of NbCr2 alloyed by X (V, Mo, Ti, Fe). Solid State Communications, 2022, 344, 114664.	1.9	1
4	Study on the structural, mechanical, and dynamical stabilities and properties of Nb₂AN (AÂ=ÂSi, Ge, and Sn) MAX phases by first principle. Journal of the American Ceramic Society, 2022, 105, 5285-5298.	3.8	4
5	Spinodal limits of supercooled liquid Al deduced from configuration heredity of crystal clusters. Computational Materials Science, 2022, 207, 111316.	3.0	3
6	Cu-induced enhancement of interfacial bonding for brazed diamond grits with Ni Cr filler alloys. International Journal of Refractory Metals and Hard Materials, 2022, 106, 105874.	3.8	8
7	Laser in-situ preparation and mechanical properties of VC reinforced Fe-based wear-resistant composite cladding. Ceramics International, 2022, 48, 28240-28249.	4.8	18
8	Theory-guided construction of electron-deficient sites via removal of lattice oxygen for the boosted electrocatalytic synthesis of ammonia. Nano Research, 2021, 14, 1457-1464.	10.4	10
9	Hydrogen storage properties and mechanisms of as-cast, homogenized and ECAP processed Mg98.5Y1Zn0.5 alloys containing LPSO phase. Energy, 2021, 217, 119315.	8.8	22
10	Micromechanism in fracture toughness of NbCr2 laves phase improved by nickel alloying: first-principles calculation. Journal of Alloys and Compounds, 2021, 857, 158040.	5.5	8
11	Stabilization of low-valence transition metal towards advanced catalytic effects on the hydrogen storage performance of magnesium hydride. Journal of Magnesium and Alloys, 2021, 9, 647-657.	11.9	53
12	Hydrogen-substituted graphdiyne/graphene as an sp/sp² hybridized carbon interlayer for lithiumâ€“sulfur batteries. Nanoscale, 2021, 13, 3817-3826.	5.6	27
13	Insight into the surface activity of defect structure in Î±-MnO2 nanorod: first-principles research. Scientific Reports, 2021, 11, 4751.	3.3	0
14	Identification of critical nuclei in the rapid solidification via configuration heredity. Journal of Physics Condensed Matter, 2021, 33, 175701.	1.8	1
15	Effect of intrinsic point-defect complex on elastic properties of Î³â€²-Ni3Al phases. Materials Research Express, 2021, 8, 066517.	1.6	1
16	Nanometer effect promoting arsenic removal on Î±-MnO2 nano-surface in aqueous solution: DFT+U research. Environmental Science and Pollution Research, 2021, 28, 65899-65910.	5.3	1
17	Impact of replacement of Re by W on dislocation slip mediated creeps of Î³â€²-Ni3Al phases. Transactions of Nonferrous Metals Society of China, 2021, 31, 2013-2023.	4.2	7
18	Effects of Ce and La elements on interfacial bonding, thermal damage and mechanical performance of brazed diamonds with Ni Cr filler alloy. International Journal of Refractory Metals and Hard Materials, 2021, 98, 105571.	3.8	14

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19	Filings Morphology-Dependent Hydrogen Storage Properties of Magnesium-Rich Mgâ€“Yâ€“Zn Alloy. Transactions of the Indian Institute of Metals, 2021, 74, 3171-3184.	1.5	2
20	Doped effect of Gd and Y elements on corrosion resistance of ZrO2 in CMAS melt: First-principles and experimental study. Journal of the European Ceramic Society, 2021, 41, 7893-7901.	5.7	13
21	Effect of Er dopant on the corrosion resistance of YSZ in CMAS melt: experimental and first-principles study. Journal of Materials Science, 2021, 56, 17542-17555.	3.7	4
22	Effect of Fe doping on structural, elastic and electronic properties of B2â€“ZrCu phase under hydrostatic pressure: A first-principles study. Materials Chemistry and Physics, 2021, 272, 124978.	4.0	3
23	Lowest-energy structural and electronic properties of Cu Zr13â^' (nÂ=Â3â€“10) clusters in metallic glasses via CALYPSO search and density functional theory calculations. Journal of Molecular Liquids, 2021, 343, 117603.	4.9	9
24	Impact of Re-clustering on resistances to dislocation slip mediated plastic deformations in Î³ matrix phases. Computational Materials Science, 2020, 172, 109314.	3.0	6
25	Bismuthene from sonoelectrochemistry as a superior anode for potassium-ion batteries. Journal of Materials Chemistry A, 2020, 8, 453-460.	10.3	94
26	Adsorption and diffusion behaviors of Ni-based filler elements on diamond surface. Journal of Alloys and Compounds, 2020, 822, 153652.	5.5	25
27	Different structural transitions of rapidly supercooled tantalum melt under pressure. Physical Chemistry Chemical Physics, 2020, 22, 18078-18090.	2.8	9
28	Cyclic oxidation behavior of NiCoCrAlY/YSZ@Ni composite coatings fabricated by laser cladding. Journal of Iron and Steel Research International, 2020, 27, 1226-1235.	2.8	4
29	Infiltration mechanism of Ca-Mg-Al-silicate (CMAS) melt on Yttria stabilized zirconia (YSZ) columnar crystal at high temperature: First-principles research. Applied Surface Science, 2020, 513, 145712.	6.1	10
30	Nearly golden-ratio order in Ta metallic glass*. Chinese Physics B, 2020, 29, 046105.	1.4	4
31	First-principles investigation on electronic structure and solar radiation shielding performance of Tl_{0.33}WO₃. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 047102.	0.5	0
32	Monolayer Phosphoreneâ€“Carbon Nanotube Heterostructures for Photocatalysis: Analysis by Density Functional Theory. Nanoscale Research Letters, 2019, 14, 233.	5.7	10
33	Interfacial bonding mechanism and adhesive transfer of brazed diamond with Ni-based filler alloy: First-principles and experimental perspective. Carbon, 2019, 153, 104-115.	10.3	63
34	Atomic structure insight into crystallization of undercooled liquid metal Zr during isothermal relaxation processes. Philosophical Magazine, 2019, 99, 2904-2919.	1.6	4
35	A synergistic reinforcement of Re and W for ideal shear strengths of Î³â€²-Ni3Al phases. Journal of Physics and Chemistry of Solids, 2019, 131, 34-43.	4.0	18
36	Wetting mechanism of CMAS melt on YSZ surface at high temperature: First-principles calculation. Applied Surface Science, 2019, 483, 811-818.	6.1	27

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37	The short-range order in liquid and A15 crystal of zirconium. Journal of Non-Crystalline Solids, 2019, 513, 111-119.	3.1	32
38	Enhanced permeability of rGO/S-GO layered membranes with tunable inter-structure for effective rejection of salts and dyes. Separation and Purification Technology, 2019, 220, 309-319.	7.9	51
39	Copperâ€Catalyzed Oxidative C(sp³)â^'H/Nâ^'H Crossâ€Coupling of Hydrocarbons with P(O)â^'NH Compounds: the Accelerating Effect Induced by Carboxylic Acid Coproduct. Advanced Synthesis and Catalysis, 2019, 361, 1689-1696.	4.3	1
40	Predictions of electronic structures and optical performance of potential near infrared absorber Sn0.33WO3. AIP Advances, 2019, 9, 115014.	1.3	4
41	Study on the surface activity of t-YSZ nanomaterials by first-principles calculation. Applied Surface Science, 2019, 471, 1072-1082.	6.1	5
42	Novel â€œlooseâ€•GO/MoS2 composites membranes with enhanced permeability for effective salts and dyes rejection at low pressure. Journal of Membrane Science, 2019, 574, 112-123.	8.2	147
43	Reduced Graphene Oxideâ€“Refined Cu Matrix Composites: An Experimental and Firstâ€Principles Study. Crystal Research and Technology, 2019, 54, 1800191.	1.3	3
44	Insights Into Interfacial Interaction and Its Influence on the Electronic and Optical Properties of Twoâ€Dimensional WS₂/TX₂CO₂ (TXâ€‰=â€‰Ti, Zr) van der Waals Heterostructures. Physica Status Solidi (B): Basic Research, 2019, 256, 1800377.	1.5	2
45	Identification and tracking of different types of crystalline nucleiduring isothermal crystallization of amorphous Ag. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 076401.	0.5	3
46	Electronic structures and optical properties of Ce-doped anatase TiO₂ with oxygen vacancy. Wuli Xuebao/Acta Physica Sinica, 2019, 68, 037101.	0.5	3
47	Effects of high pressure on microstructure evolution and crystallization mechanisms during solidification of nickel. Materials Research Express, 2018, 5, 036507.	1.6	4
48	Interfacial Interaction between Boron Cluster and Metal Oxide Surface and Its Effects: A Case Study of B₂₀/Ag₃PO₄ van der Waals Heterostructure. Journal of Physical Chemistry C, 2018, 122, 6151-6158.	3.1	7
49	Research on the removal mechanism of antimony on Î±-MnO2 nanorod in aqueous solution: DFTâ€+â€U method. Journal of Hazardous Materials, 2018, 354, 8-16.	12.4	22
50	Correlation between the chemical order and nature property of Cu-centered Cu-Zr icosahedral clusters. Materials Research Express, 2018, 5, 046302.	1.6	3
51	Derivative effect of laser cladding on interface stability of YSZ@Ni coating on GH4169 alloy: An experimental and theoretical study. Applied Surface Science, 2018, 427, 1105-1113.	6.1	9
52	Arsenic adsorption on Î±-MnO2 nanofibers and the significance of (1 0 0) facet as compared with (1 1 0). Chemical Engineering Journal, 2018, 331, 492-500.	12.7	106
53	Interfacial Interactions in Monolayer and Fewâ€Layer SnS/CH₃NH₃PbI₃ Perovskite van der Waals Heterostructures and Their Effects on Electronic and Optical Properties. ChemPhysChem, 2018, 19, 291-299.	2.1	12
54	Effect of P-Doping on the Rupture Strength of Î³-Ni/Î³'-Ni3Al Interfaces. IOP Conference Series: Materials Science and Engineering, 2018, 381, 012161.	0.6	2

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55	Theory-Driven Heterojunction Photocatalyst Design with Continuously Adjustable Band Gap Materials. Journal of Physical Chemistry C, 2018, 122, 28065-28074.	3.1	20
56	Cs0.33WO3 as a high-performance transparent solar radiation shielding material for windows. Journal of Applied Physics, 2018, 124, .	2.5	14
57	Enhanced hydrogen storage properties and mechanisms of magnesium hydride modified by transition metal dissolved magnesium oxides. International Journal of Hydrogen Energy, 2018, 43, 21864-21873.	7.1	31
58	Evolution of local atomic structures during rapid solidification of liquid metal W. Modern Physics Letters B, 2018, 32, 1850368.	1.9	4
59	In Situ Tuning of Catalytic Activity by Thermoelectric Effect for Ethylene Oxidation. ACS Catalysis, 2018, 8, 10164-10172.	11.2	20
60	Impact of correlative defects induced by double Re-addition on the ideal shear strength of Î³â€²-Ni3Al phases. Computational Materials Science, 2018, 152, 408-416.	3.0	19
61	Evolution Mechanism of Metallic Dioxide MO2 (M = Mn, Ti) from Nanorods to Bulk Crystal: First-Principles Research. Journal of Nanomaterials, 2018, 2018, 1-14.	2.7	3
62	Mechanism of crack nucleation and growth in YSZ thermal barrier coatings corroded by CMAS at high temperatures: First-principles calculation. Corrosion Science, 2018, 142, 258-265.	6.6	25
63	Simultaneous dispersive and covalent monolayer MoS2/TiO2 cluster heterostructures: Insights into their enhanced photocatalytic activity. Superlattices and Microstructures, 2018, 121, 64-74.	3.1	0
64	Local atomic structures of amorphous Pd₈₀Si₂₀ alloys and their configuration heredity in the rapid solidification. Philosophical Magazine, 2018, 98, 2861-2877.	1.6	9
65	Correlation between the chemical short-range order and binding energy of Cu-centred CunZr13â^'n(nÂ=Â6,7,8,9) icosahedral clusters in metallic glass. Molecular Simulation, 2018, 44, 1183-1190.	2.0	4
66	Tuning the near-gap electronic structure of Cu2O by anionâ€“cation co-doping for enhanced solar energy conversion. Modern Physics Letters B, 2017, 31, 1650429.	1.9	4
67	Electronic and optical properties of Cr-, B-doped, and (Cr, B)-codoped SrTiO₃. International Journal of Modern Physics B, 2017, 31, 1750064.	2.0	2
68	A DFT study on the competition and evolution characteristics between icosahedra and FCC clusters in rapid solidification of liquid Ag. Journal of Molecular Liquids, 2017, 230, 271-279.	4.9	7
69	Simultaneous covalent and noncovalent carbon nanotube/Ag₃PO₄ hybrids: new insights into the origin of enhanced visible light photocatalytic performance. Physical Chemistry Chemical Physics, 2017, 19, 7955-7963.	2.8	13
70	High-temperature oxidation resistance of the Ni60Ti alloy: An experimental and first-principles study. Journal of Alloys and Compounds, 2017, 706, 297-304.	5.5	9
71	Hybrid TiO₂/graphene derivatives nanocomposites: is functionalized graphene better than pristine graphene for enhanced photocatalytic activity?. Catalysis Science and Technology, 2017, 7, 1423-1432.	4.1	20
72	Antimony Removal from Aqueous Solution Using Novel Î±-MnO₂ Nanofibers: Equilibrium, Kinetic, and Density Functional Theory Studies. ACS Sustainable Chemistry and Engineering, 2017, 5, 2255-2264.	6.7	85

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73	Structural evolutions and hereditary characteristics of icosahedral nano-clusters formed in Mg70Zn30 alloys during rapid solidification processes. Scientific Reports, 2017, 7, 43111.	3.3	11
74	Alkali metal silanides Î±-MSiH3: A family of complex hydrides for solid-state hydrogen storage. International Journal of Hydrogen Energy, 2017, 42, 12405-12413.	7.1	15
75	Effects of pressure on microstructure evolution and mechanical properties of liquid Ni64Zr36 alloy during rapid solidification: A molecular dynamics simulation study. Computational Materials Science, 2017, 137, 30-38.	3.0	8
76	Effect of high pressure on the formation and evolution of clusters during the rapid solidification of zirconium melts. Computational Materials Science, 2017, 140, 275-283.	3.0	21
77	Noncovalent Functionalization of Monolayer MoS₂ with Carbon Nanotubes: Tuning Electronic Structure and Photocatalytic Activity. Journal of Physical Chemistry C, 2017, 121, 21921-21929.	3.1	23
78	High-temperature corrosion mechanism of YSZ coatings subject to calciumâ€“magnesiumâ€“aluminosilicate (CMAS) deposits: First-principles calculations. Corrosion Science, 2017, 126, 286-294.	6.6	47
79	The mechanism of enhanced photocatalytic activity of SnO 2 through fullerene modification. Current Applied Physics, 2017, 17, 1547-1556.	2.4	14
80	First-principles study of electronic, mechanical and optical properties of mixed valence SmB6. IOP Conference Series: Materials Science and Engineering, 2017, 207, 012084.	0.6	3
81	Mechanism of surface effect and selective catalytic performance of MnO 2 nanorod: DFT+U study. Applied Surface Science, 2017, 420, 205-213.	6.1	19
82	Enhanced hydrogen diffusion in magnesium based hydride induced by strain and doping from first principle study. Journal of Alloys and Compounds, 2017, 694, 687-693.	5.5	18
83	A comparative study on local atomic configurations characterized by cluster-type-index method and Voronoi polyhedron method. Computational Materials Science, 2016, 123, 214-223.	3.0	35
84	First-principles investigation on solar radiation shielding performance of rutile VO2 filters for smart windows. Applied Physics Letters, 2016, 109, .	3.3	10
85	First-principles prediction of solar radiation shielding performance for transparent windows of GdB6. Journal of Applied Physics, 2016, 119, .	2.5	14
86	Dual role of monolayer MoS2 in enhanced photocatalytic performance of hybrid MoS2/SnO2 nanocomposite. Journal of Applied Physics, 2016, 119, .	2.5	57
87	Near-infrared radiation absorption properties of covellite (CuS) using first-principles calculations. AIP Advances, 2016, 6, .	1.3	21
88	Investigation on the electronic structures and optical performances of Siâ€“S codoped anatase TiO 2 by first-principles calculation. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 1462-1468.	2.1	10
89	Solar radiation shielding properties of transparent LaB6 filters through experimental and first-principles calculation methods. Ceramics International, 2016, 42, 14278-14281.	4.8	15
90	Electronic properties and photoactivity of monolayer MoS₂/fullerene van der Waals heterostructures. RSC Advances, 2016, 6, 43228-43236.	3.6	28

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91	Non-covalent functionalization of WS₂ monolayer with small fullerenes: tuning electronic properties and photoactivity. Dalton Transactions, 2016, 45, 13383-13391.	3.3	22
92	Dual functions of 2D WS₂and MoS₂â€“WS₂monolayers coupled with a Ag₃PO₄photocatalyst. Semiconductor Science and Technology, 2016, 31, 095013.	2.0	8
93	Predictions of solar radiation shielding properties of KB 6 from first principles. Computational Condensed Matter, 2016, 9, 1-5.	2.1	4
94	Molecular dynamics study on microstructural evolution during crystallization of rapidly supercooled zirconium melts. Journal of Alloys and Compounds, 2016, 688, 654-665.	5.5	38
95	Effective interactions and atomic ordering in Ni-rich Ni-Re alloys. Physical Review B, 2016, 94, .	3.2	19
96	Dramatically Enhanced Visible Light Response of Monolayer ZrS2 via Non-covalent Modification by Double-Ring Tubular B20 Cluster. Nanoscale Research Letters, 2016, 11, 495.	5.7	25
97	Tuning near-gap electronic structure, interface charge transfer and visible light response of hybrid doped graphene and Ag3PO4 composite: Dopant effects. Scientific Reports, 2016, 6, 22267.	3.3	24
98	Crystallization characteristics in supercooled liquid zinc during isothermal relaxation: A molecular dynamics simulation study. Scientific Reports, 2016, 6, 31653.	3.3	15
99	Theoretical analyses of organic acids assisted surface-catalyzed reduction of Cr VI on TiO 2 nanowire arrays. Applied Catalysis B: Environmental, 2016, 198, 508-515.	20.2	23
100	Enhanced photocatalytic performance of an Ag₃PO₄ photocatalyst via fullerene modification: first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 2878-2886.	2.8	22
101	Structural stability of characteristic interface for NiTi/Nb Nanowire: First-Principle study. Metals and Materials International, 2016, 22, 69-74.	3.4	5
102	Cohesive mechanism of the FeCr/Ni Interface: A first-principles study. Metals and Materials International, 2016, 22, 75-80.	3.4	5
103	Strain tuned dehydrogenation thermodynamics of magnesium based hydride: A first principle study. Computational Materials Science, 2015, 105, 71-74.	3.0	8
104	Micromechanism of Cu and Fe alloying process on the martensitic phase transformation of NiTi-based alloys: First-principles calculation. Journal of Structural Chemistry, 2015, 56, 1051-1057.	1.0	4
105	Effects of S/Ce-codoping on electronic structures and optical properties of anatase TiO2 from density functional theory calculations. Modern Physics Letters B, 2015, 29, 1550249.	1.9	1
106	Effect of cooling rates on clustering towards icosahedra in rapidly solidified Cu56Zr44 alloy. Transactions of Nonferrous Metals Society of China, 2015, 25, 533-543.	4.2	6
107	Origin of photocatalytic activity of nitrogen-doped germanium dioxide under visible light from first principles. Materials Science in Semiconductor Processing, 2015, 31, 517-524.	4.0	8
108	A DFT study on the heredity-induced coalescence of icosahedral basic clusters in the rapid solidification. Computational Materials Science, 2015, 99, 156-163.	3.0	13

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109	Electronic Structures and Photocatalytic Responses of SrTiO₃(100) Surface Interfaced with Graphene, Reduced Graphene Oxide, and Graphane: Surface Termination Effect. Journal of Physical Chemistry C, 2015, 119, 19095-19104.	3.1	32
110	Phase stability, elastic properties and electronic structures of Mgâ€“Y intermetallics from first-principles calculations. Journal of Magnesium and Alloys, 2015, 3, 127-133.	11.9	27
111	Enhancement of transport properties introduced complex defect in (6, 3) carbon nanotubes. Modern Physics Letters B, 2015, 29, 1550031.	1.9	0
112	Non-linear effects of initial melt temperatures on microstructures and mechanical properties during quenching process of liquid Cu46Zr54 alloy. Physica B: Condensed Matter, 2015, 465, 81-88.	2.7	4
113	Optical transportation and controllable positioning of nanospheres using a microfiber. AIP Advances, 2015, 5, .	1.3	5
114	Correlation of the heredity of icosahedral clusters with the glass forming ability of rapidly solidified Cu x Zr 100â^'x alloys. Journal of Non-Crystalline Solids, 2015, 427, 199-207.	3.1	24
115	Band structure engineering of monolayer MoS₂: a charge compensated codoping strategy. RSC Advances, 2015, 5, 7944-7952.	3.6	26
116	Dehydrogenation thermodynamics of magnesium hydride doped with transition metals: Experimental and theoretical studies. Computational Materials Science, 2015, 98, 211-219.	3.0	32
117	Magnetic properties of NI-doped ZnS: First-principles study. Journal of Magnetism and Magnetic Materials, 2015, 377, 239-242.	2.3	21
118	Formation and evolution of nano-clusters in a large-scale system of Cuâ€“Zr alloy during rapid solidification process. Computational Materials Science, 2015, 98, 1-9.	3.0	15
119	THE ELECTRONIC AND OPTICAL PROPERTIES OF X-DOPED SrTiO₃ (X = Rh, Pd,) Tj ETQq1 1 0.784314 rgBT /O	2.0	8
120	Negative differential resistance induced by SiNx co-dopant in armchair graphene nanoribbon. Modern Physics Letters B, 2014, 28, 1450229.	1.9	3
121	Diverse and tunable electronic structures of single-layer metal phosphorus trichalcogenides for photocatalytic water splitting. Journal of Chemical Physics, 2014, 140, 054707.	3.0	99
122	Electronic structures and optical properties of two-dimensional ScN and YN nanosheets. Journal of Applied Physics, 2014, 115, .	2.5	30
123	Nb solution influencing on phase transformation temperature of Ni47Ti44Nb9 alloy. Journal of Alloys and Compounds, 2014, 609, 156-161.	5.5	24
124	First-principles investigation of the binary intermetallics in Mgâ€“Alâ€“Sr alloy: Stability, elastic properties and electronic structure. Computational Materials Science, 2014, 86, 24-29.	3.0	36
125	Band engineering of ZnS by codoping for visible-light photocatalysis. Applied Physics A: Materials Science and Processing, 2014, 116, 741-750.	2.3	32
126	Band gap engineering by lanthanide doping in the photocatalyst LaOF: First-principles study. International Journal of Modern Physics B, 2014, 28, 1450069.	2.0	6

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127	Single-layer Group-IVB nitride halides as promising photocatalysts. Journal of Materials Chemistry A, 2014, 2, 6755.	10.3	90
128	Native vacancy defects in bismuth sulfide. International Journal of Modern Physics B, 2014, 28, 1450150.	2.0	15
129	An interplay of sulfur and phosphorus at the Î³-Ni/Î³â€²-Ni3Al interface. Journal of Alloys and Compounds, 2014, 597, 243-248.	5.5	21
130	The effect of cooling rates on hereditary characteristics of icosahedral clusters in rapid solidification of liquid Cu56Zr44 alloys. Journal of Non-Crystalline Solids, 2014, 388, 75-85.	3.1	16
131	Mechanism of Superior Visible-Light Photocatalytic Activity and Stability of Hybrid Ag₃PO₄/Graphene Nanocomposite. Journal of Physical Chemistry C, 2014, 118, 12972-12979.	3.1	78
132	Influence of icosahedral order on the second peak splitting of pair distribution function for Mg70Zn30 metallic glass. Journal of Alloys and Compounds, 2014, 597, 269-274.	5.5	45
133	Band-Gap Widening of Nitrogen-Doped Cu₂O: New Insights from First-Principles Calculations. Science of Advanced Materials, 2014, 6, 1221-1227.	0.7	10
134	Strain effect on structural and dehydrogenation properties of MgH2 hydride from first-principles calculations. International Journal of Hydrogen Energy, 2013, 38, 3661-3669.	7.1	41
135	On the heredity and evolution of icosahedral clusters during the rapid solidification of liquid Cu50Zr50 alloys. Journal of Non-Crystalline Solids, 2013, 378, 61-70.	3.1	27
136	Simulation study on non-linear effects of initial melt temperatures on microstructures during solidification process of liquid Mg7Zn3 alloy. Transactions of Nonferrous Metals Society of China, 2013, 23, 1052-1060.	4.2	10
137	Enhancement of the hole-induced d⁰-ferromagnetism in ZnO through compensated donorâ€“acceptor complexes: a first-principles study. Semiconductor Science and Technology, 2013, 28, 035017.	2.0	8
138	Rectifying behaviors introduced by nitrogen-vacancy complex in spiral chirality single walled carbon nanotube device. Journal of Applied Physics, 2013, 114, .	2.5	1
139	TUNING THE "d⁰" FERROMAGNETISM IN In₂O₃ QUANTUM DOTS BY DANGLING BONDS AND VACANCY BASED ON THE FIRST-PRINCIPLE CALCULATION. Modern Physics Letters B, 2013, 27, 1350068.	1.9	7
140	Optical and Electronic Properties of Ni-Doped ZnS: First-Principles Study. Journal of Nanoelectronics and Optoelectronics, 2013, 8, 297-301.	0.5	1
141	A TS Search for Stable Configurations of Double Icosahedral Agn(n=19, 23, 24, 25) Clusters Linked by Sharing Atoms. Acta Chimica Sinica, 2013, 71, 1429.	1.4	3
142	Microcosmic mechanism of carbon influencing on NiTiNb9 alloy. Journal of Alloys and Compounds, 2012, 542, 170-176.	5.5	22
143	Origins of high visible light transparency and solar heat-shielding performance in LaB₆. Applied Physics Letters, 2012, 101, 041913.	3.3	62
144	Microstructural evolution and martensitic transformation mechanisms during solidification processes of liquid metal Pb. Philosophical Magazine, 2012, 92, 571-585.	1.6	10

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145	Synergistic effect of Ti and F co-doping on dehydrogenation properties of MgH2 from first-principles calculations. Journal of Alloys and Compounds, 2012, 538, 205-211.	5.5	35
146	The correlation between Re and P and their synergetic effect on the rupture strength of the Î³-Ni/Î³â€²-Ni3Al interface. Computational Materials Science, 2012, 63, 292-302.	3.0	21
147	Thermal stability and elastic properties of Mg2X (X = Si, Ge, Sn, Pb) phases from first-principle calculations. Computational Materials Science, 2012, 51, 409-414.	3.0	86
148	Structural, elastic and electronic properties of Î¸ (Al2Cu) and S (Al2CuMg) strengthening precipitates in Alâ€“Cuâ€“Mg series alloys: First-principles calculations. Solid State Communications, 2012, 152, 2100-2104.	1.9	105
149	Electronic and optical properties of vacancy-doped WS2 monolayers. AIP Advances, 2012, 2, .	1.3	41
150	Firstâ€principles investigation of H₂O adsorption on a BN coâ€doped nanotube. Physica Status Solidi (B): Basic Research, 2012, 249, 69-73.	1.5	2
151	Kinetic details of crystallization in supercooled liquid Pb during the isothermal relaxation. Physica B: Condensed Matter, 2012, 407, 240-245.	2.7	13
152	First-Principles Calculation on Dehydrogenating Properties of LiBH4-X(X¼O,F,Cl)Systems. Acta Chimica Sinica, 2012, 70, 71.	1.4	2
153	MOLECULAR DYNAMICS SIMULATION ON THE EVOLUTION OF MICROSTRUCTURES OF LIQUID ZnxAl100?x ALLOYS DURING RAPID SOLIDIFICATION. Jinshu Xuebao/Acta Metallurgica Sinica, 2012, 48, 907.	0.3	0
154	Study on the electronic structure and the optical performance of YB6 by the first-principles calculations. AIP Advances, 2011, 1, .	1.3	12
155	A first-principles study on electronic structure and elastic properties of Al4Sr, Mg2Sr and Mg23Sr6 phases. Transactions of Nonferrous Metals Society of China, 2011, 21, 2677-2683.	4.2	10
156	Ab initio calculations on energetics and electronic structures of cubic Mg3MNi2 (MÂ=ÂAl, Ti, Mn) hydrogen storage alloys. International Journal of Hydrogen Energy, 2011, 36, 14477-14483.	7.1	19
157	Research progress in LiBH4 for hydrogen storage: A review. International Journal of Hydrogen Energy, 2011, 36, 14512-14526.	7.1	154
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