Ping Peng

List of Publications by Year in Descending Order

196 papers	3,098 citations	30 h-index	44 g-index
203 ext. papers	3,636 ext. citations	3.8 avg, IF	5.34 L-index

#	Paper	IF	Citations
196	First-principles investigations of the fracture toughness of NbCr2 alloyed by X (V, Mo, Ti, Fe). *Solid State Communications*, **2022**, 344, 114664	1.6	
195	Competition between TCP and crystalline clusters during phase transition of rapidly super-cooled aluminum. *Journal of Non-Crystalline Solids*, **2022**, 576, 121271	3.9	2
194	Spinodal limits of supercooled liquid Al deduced from configuration heredity of crystal clusters. *Computational Materials Science*, **2022**, 207, 111316	3.2	0
193	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	4.1	0
192	Effect of intrinsic point-defect complex on elastic properties of γ′-Ni3Al phases. *Materials Research Express*, **2021**, 8, 066517	1.7	
191	Nanometer effect promoting arsenic removal on δ-MnO nano-surface in aqueous solution: DFT+U research. *Environmental Science and Pollution Research*, **2021**, 28, 65899-65910	5.1	
190	Impact of replacement of Re by W on dislocation slip mediated creeps of γ′-Ni3Al phases. *Transactions of Nonferrous Metals Society of China*, **2021**, 31, 2013-2023	3.3	0
189	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	2
188	Hydrogen storage properties and mechanisms of as-cast, homogenized and ECAP processed Mg98.5Y1Zn0.5 alloys containing LPSO phase. *Energy*, **2021**, 217, 119315	7.9	6
187	Micromechanism in fracture toughness of NbCr2 laves phase improved by nickel alloying: first-principles calculation. *Journal of Alloys and Compounds*, **2021**, 857, 158040	5.7	1
186	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	8.8	20
185	Hydrogen-substituted graphdiyne/graphene as an sp/sp hybridized carbon interlayer for lithium-sulfur batteries. *Nanoscale*, **2021**, 13, 3817-3826	7.7	12
184	Insight into the surface activity of defect structure in δ-MnO nanorod: first-principles research. *Scientific Reports*, **2021**, 11, 4751	4.9	
183	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	4.1	4
182	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, 7893-7893	6	0
181	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	4.3	1
180	Effect of Fe doping on structural, elastic and electronic properties of B2-ZrCu phase under hydrostatic pressure: A first-principles study. *Materials Chemistry and Physics*, **2021**, 272, 124978	4.4	

179	Lowest-energy structural and electronic properties of Cu Zr13−n (n = 3–10) clusters in metallic glasses via CALYPSO search and density functional theory calculations. *Journal of Molecular Liquids*, **2021**, 343, 117603	6	0
178	Cyclic oxidation behavior of NiCoCrAlY/YSZ@Ni composite coatings fabricated by laser cladding. *Journal of Iron and Steel Research International*, **2020**, 27, 1226-1235	1.2	2
177	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	6.7	7
176	Nearly golden-ratio order in Ta metallic glass. *Chinese Physics B*, **2020**, 29, 046105	1.2	1
175	First-principles investigation on electronic structure and solar radiation shielding performance of Tl0.33WO3. *Wuli Xuebao/Acta Physica Sinica*, **2020**, 69, 047102	0.6	
174	Bismuthene from sonoelectrochemistry as a superior anode for potassium-ion batteries. *Journal of Materials Chemistry A*, **2020**, 8, 453-460	13	62
173	Adsorption and diffusion behaviors of Ni-based filler elements on diamond surface. *Journal of Alloys and Compounds*, **2020**, 822, 153652	5.7	18
172	Different structural transitions of rapidly supercooled tantalum melt under pressure. *Physical Chemistry Chemical Physics*, **2020**, 22, 18078-18090	3.6	4
171	Impact of Re-clustering on resistances to dislocation slip mediated plastic deformations in γ matrix phases. *Computational Materials Science*, **2020**, 172, 109314	3.2	3
170	Atomic structure insight into crystallization of undercooled liquid metal Zr during isothermal relaxation processes. *Philosophical Magazine*, **2019**, 99, 2904-2919	1.6	1
169	A synergistic reinforcement of Re and W for ideal shear strengths of γ′-Ni3Al phases. *Journal of Physics and Chemistry of Solids*, **2019**, 131, 34-43	3.9	11
168	Wetting mechanism of CMAS melt on YSZ surface at high temperature: First-principles calculation. *Applied Surface Science*, **2019**, 483, 811-818	6.7	13
167	The short-range order in liquid and A15 crystal of zirconium. *Journal of Non-Crystalline Solids*, **2019**, 513, 111-119	3.9	18
166	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	8.3	29
165	Copper-Catalyzed Oxidative C(sp3)–H/N–H Cross-Coupling of Hydrocarbons with P(O)–N–H Compounds: the Accelerating Effect Induced by Carboxylic Acid Coproduct. *Advanced Synthesis and Catalysis*, **2019**, 361, 1689-1696	5.6	1
164	Monolayer Phosphorene-Carbon Nanotube Heterostructures for Photocatalysis: Analysis by Density Functional Theory. *Nanoscale Research Letters*, **2019**, 14, 233	5	3
163	Interfacial bonding mechanism and adhesive transfer of brazed diamond with Ni-based filler alloy: First-principles and experimental perspective. *Carbon*, **2019**, 153, 104-115	10.4	27
162	Identification and tracking of different types of crystalline nucleiduring isothermal crystallization of amorphous Ag. *Wuli Xuebao/Acta Physica Sinica*, **2019**, 68, 076401	0.6	2

161	Electronic structures and optical properties of Ce-doped anatase TiO2 with oxygen vacancy. *Wuli Xuebao/Acta Physica Sinica*, **2019**, 68, 037101	0.6	2
160	Predictions of electronic structures and optical performance of potential near infrared absorber Sn0.33WO3. *AIP Advances*, **2019**, 9, 115014	1.5	0
159	Study on the surface activity of t-YSZ nanomaterials by first-principles calculation. *Applied Surface Science*, **2019**, 471, 1072-1082	6.7	2
158	Novel □bose□GO/MoS2 composites membranes with enhanced permeability for effective salts and dyes rejection at low pressure. *Journal of Membrane Science*, **2019**, 574, 112-123	9.6	89
157	Reduced Graphene Oxide□Refined Cu Matrix Composites: An Experimental and First-Principles Study. *Crystal Research and Technology*, **2019**, 54, 1800191	1.3	0
156	Insights Into Interfacial Interaction and Its Influence on the Electronic and Optical Properties of Two-Dimensional WS2/TX2CO2 (TX = Ti, Zr) van der Waals Heterostructures. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800377	1.3	1
155	Effects of high pressure on microstructure evolution and crystallization mechanisms during solidification of nickel. *Materials Research Express*, **2018**, 5, 036507	1.7	3
154	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	3.8	7
153	Research on the removal mechanism of antimony on □MnO nanorod in aqueous solution: DFT + U method. *Journal of Hazardous Materials*, **2018**, 354, 8-16	12.8	17
152	Correlation between the chemical order and nature property of Cu-centered Cu-Zr icosahedral clusters. *Materials Research Express*, **2018**, 5, 046302	1.7	2
151	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	6.7	6
150	Arsenic adsorption on □MnO2 nanofibers and the significance of (1 0 0) facet as compared with (1 1 0). *Chemical Engineering Journal*, **2018**, 331, 492-500	14.7	56
149	Impact of correlative defects induced by double Re-addition on the ideal shear strength of □-Ni3Al phases. *Computational Materials Science*, **2018**, 152, 408-416	3.2	9
148	Evolution Mechanism of Metallic Dioxide MO2 (M = Mn, Ti) from Nanorods to Bulk Crystal: First-Principles Research. *Journal of Nanomaterials*, **2018**, 2018, 1-14	3.2	3
147	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	6.8	14
146	Simultaneous dispersive and covalent monolayer MoS2/TiO2 cluster heterostructures: Insights into their enhanced photocatalytic activity. *Superlattices and Microstructures*, **2018**, 121, 64-74	2.8	
145	Local atomic structures of amorphous Pd80Si20 alloys and their configuration heredity in the rapid solidification. *Philosophical Magazine*, **2018**, 98, 2861-2877	1.6	4
144	Correlation between the chemical short-range order and binding energy of Cu-centred CunZr13□(n = 6,7,8,9) icosahedral clusters in metallic glass. *Molecular Simulation*, **2018**, 44, 1183-1190	2	3

143	Interfacial Interactions in Monolayer and Few-Layer SnS/CH NH PbI Perovskite van der Waals Heterostructures and Their Effects on Electronic and Optical Properties. *ChemPhysChem*, **2018**, 19, 291-299	3.2	12
142	Effect of P-Doping on the Rupture Strength of Ni/Ni3Al Interfaces. *IOP Conference Series: Materials Science and Engineering*, **2018**, 381, 012161	0.4	2
141	Theory-Driven Heterojunction Photocatalyst Design with Continuously Adjustable Band Gap Materials. *Journal of Physical Chemistry C*, **2018**, 122, 28065-28074	3.8	17
140	Cs0.33WO3 as a high-performance transparent solar radiation shielding material for windows. *Journal of Applied Physics*, **2018**, 124, 193102	2.5	6
139	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	6.7	21
138	Study of Processability of Cu/Ni Bilayers Using Molecular Dynamics Simulations. *Journal of Nano Research*, **2018**, 52, 43-53	1	1
137	Evolution of local atomic structures during rapid solidification of liquid metal W. *Modern Physics Letters B*, **2018**, 32, 1850368	1.6	2
136	In Situ Tuning of Catalytic Activity by Thermoelectric Effect for Ethylene Oxidation. *ACS Catalysis*, **2018**, 8, 10164-10172	13.1	10
135	Tuning the near-gap electronic structure of Cu2O by anion ation co-doping for enhanced solar energy conversion. *Modern Physics Letters B*, **2017**, 31, 1650429	1.6	4
134	Electronic and optical properties of Cr-, B-doped, and (Cr, B)-codoped SrTiO3. *International Journal of Modern Physics B*, **2017**, 31, 1750064	1.1	1
133	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	6	4
132	Simultaneous covalent and noncovalent carbon nanotube/AgPO hybrids: new insights into the origin of enhanced visible light photocatalytic performance. *Physical Chemistry Chemical Physics*, **2017**, 19, 7955-7963	3.6	11
131	High-temperature oxidation resistance of the Ni60Ti alloy: An experimental and first-principles study. *Journal of Alloys and Compounds*, **2017**, 706, 297-304	5.7	6
130	Hybrid TiO2/graphene derivatives nanocomposites: is functionalized graphene better than pristine graphene for enhanced photocatalytic activity?. *Catalysis Science and Technology*, **2017**, 7, 1423-1432	5.5	17
129	Antimony Removal from Aqueous Solution Using Novel MnO2 Nanofibers: Equilibrium, Kinetic, and Density Functional Theory Studies. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 2255-2264	8.3	60
128	Structural evolutions and hereditary characteristics of icosahedral nano-clusters formed in MgZn alloys during rapid solidification processes. *Scientific Reports*, **2017**, 7, 43111	4.9	8
127	Alkali metal silanides MSiH3: A family of complex hydrides for solid-state hydrogen storage. *International Journal of Hydrogen Energy*, **2017**, 42, 12405-12413	6.7	9
126	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	3.2	6

125	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	3.2	15
124	Noncovalent Functionalization of Monolayer MoS2 with Carbon Nanotubes: Tuning Electronic Structure and Photocatalytic Activity. *Journal of Physical Chemistry C*, **2017**, 121, 21921-21929	3.8	19
123	High-temperature corrosion mechanism of YSZ coatings subject to calciumBmagnesiumBluminosilicate (CMAS) deposits: First-principles calculations. *Corrosion Science*, **2017**, 126, 286-294	6.8	30
122	The mechanism of enhanced photocatalytic activity of SnO2 through fullerene modification. *Current Applied Physics*, **2017**, 17, 1547-1556	2.6	11
121	First-principles study of electronic, mechanical and optical properties of mixed valence SmB6. *IOP Conference Series: Materials Science and Engineering*, **2017**, 207, 012084	0.4	3
120	Mechanism of surface effect and selective catalytic performance of MnO 2 nanorod: DFT+U study. *Applied Surface Science*, **2017**, 420, 205-213	6.7	15
119	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	5.7	14
118	Dual functions of 2D WS2and MoS2WS2monolayers coupled with a Ag3PO4photocatalyst. *Semiconductor Science and Technology*, **2016**, 31, 095013	1.8	5
117	Predictions of solar radiation shielding properties of KB6 from first principles. *Computational Condensed Matter*, **2016**, 9, 1-5	1.7	2
116	Molecular dynamics study on microstructural evolution during crystallization of rapidly supercooled zirconium melts. *Journal of Alloys and Compounds*, **2016**, 688, 654-665	5.7	29
115	Effective interactions and atomic ordering in Ni-rich Ni-Re alloys. *Physical Review B*, **2016**, 94,	3.3	13
114	Dramatically Enhanced Visible Light Response of Monolayer ZrS via Non-covalent Modification by Double-Ring Tubular B Cluster. *Nanoscale Research Letters*, **2016**, 11, 495	5	16
113	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	4.9	19
112	Crystallization characteristics in supercooled liquid zinc during isothermal relaxation: A molecular dynamics simulation study. *Scientific Reports*, **2016**, 6, 31653	4.9	13
111	Theoretical analyses of organic acids assisted surface-catalyzed reduction of CrVI on TiO2 nanowire arrays. *Applied Catalysis B: Environmental*, **2016**, 198, 508-515	21.8	21
110	Enhanced photocatalytic performance of an Ag3PO4 photocatalyst via fullerene modification: first-principles study. *Physical Chemistry Chemical Physics*, **2016**, 18, 2878-86	3.6	22
109	Structural stability of characteristic interface for NiTi/Nb Nanowire: First-Principle study. *Metals and Materials International*, **2016**, 22, 69-74	2.4	4
108	Cohesive mechanism of the FeCr/Ni Interface: A first-principles study. *Metals and Materials International*, **2016**, 22, 75-80	2.4	4

107	A comparative study on local atomic configurations characterized by cluster-type-index method and Voronoi polyhedron method. *Computational Materials Science*, **2016**, 123, 214-223	3.2	28
106	First-principles investigation on solar radiation shielding performance of rutile VO2 filters for smart windows. *Applied Physics Letters*, **2016**, 109, 193906	3.4	8
105	First-principles prediction of solar radiation shielding performance for transparent windows of GdB6. *Journal of Applied Physics*, **2016**, 119, 164903	2.5	10
104	Dual role of monolayer MoS2 in enhanced photocatalytic performance of hybrid MoS2/SnO2 nanocomposite. *Journal of Applied Physics*, **2016**, 119, 205704	2.5	49
103	Near-infrared radiation absorption properties of covellite (CuS) using first-principles calculations. *AIP Advances*, **2016**, 6, 085122	1.5	17
102	Investigation on the electronic structures and optical performances of Si□ codoped anatase TiO 2 by first-principles calculation. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2016**, 380, 1462-1468	2.3	8
101	Solar radiation shielding properties of transparent LaB6 filters through experimental and first-principles calculation methods. *Ceramics International*, **2016**, 42, 14278-14281	5.1	13
100	Electronic properties and photoactivity of monolayer MoS2/fullerene van der Waals heterostructures. *RSC Advances*, **2016**, 6, 43228-43236	3.7	26
99	Non-covalent functionalization of WS2 monolayer with small fullerenes: tuning electronic properties and photoactivity. *Dalton Transactions*, **2016**, 45, 13383-91	4.3	20
98	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	3.8	29
97	Phase stability, elastic properties and electronic structures of Mg□ intermetallics from first-principles calculations. *Journal of Magnesium and Alloys*, **2015**, 3, 127-133	8.8	15
96	Enhancement of transport properties introduced complex defect in (6, 3) carbon nanotubes. *Modern Physics Letters B*, **2015**, 29, 1550031	1.6	
95	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	2.8	4
94	Optical transportation and controllable positioning of nanospheres using a microfiber. *AIP Advances*, **2015**, 5, 037126	1.5	3
93	Correlation of the heredity of icosahedral clusters with the glass forming ability of rapidly solidified CuxZr100 □x alloys. *Journal of Non-Crystalline Solids*, **2015**, 427, 199-207	3.9	17
92	Band structure engineering of monolayer MoS2: a charge compensated codoping strategy. *RSC Advances*, **2015**, 5, 7944-7952	3.7	24
91	Dehydrogenation thermodynamics of magnesium hydride doped with transition metals: Experimental and theoretical studies. *Computational Materials Science*, **2015**, 98, 211-219	3.2	26
90	Magnetic properties of NI-doped ZnS: First-principles study. *Journal of Magnetism and Magnetic Materials*, **2015**, 377, 239-242	2.8	17

89	Formation and evolution of nano-clusters in a large-scale system of Cu□r alloy during rapid solidification process. *Computational Materials Science*, **2015**, 98, 1-9	3.2	15
88	Strain tuned dehydrogenation thermodynamics of magnesium based hydride: A first principle study. *Computational Materials Science*, **2015**, 105, 71-74	3.2	5
87	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	0.9	3
86	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	1.6	1
85	Effect of cooling rates on clustering towards icosahedra in rapidly solidified Cu56Zr44 alloy. *Transactions of Nonferrous Metals Society of China*, **2015**, 25, 533-543	3.3	6
84	Origin of photocatalytic activity of nitrogen-doped germanium dioxide under visible light from first principles. *Materials Science in Semiconductor Processing*, **2015**, 31, 517-524	4.3	7
83	A DFT study on the heredity-induced coalescence of icosahedral basic clusters in the rapid solidification. *Computational Materials Science*, **2015**, 99, 156-163	3.2	10
82	Band engineering of ZnS by codoping for visible-light photocatalysis. *Applied Physics A: Materials Science and Processing*, **2014**, 116, 741-750	2.6	30
81	Band gap engineering by lanthanide doping in the photocatalyst LaOF: First-principles study. *International Journal of Modern Physics B*, **2014**, 28, 1450069	1.1	3
80	Single-layer Group-IVB nitride halides as promising photocatalysts. *Journal of Materials Chemistry A*, **2014**, 2, 6755	13	69
79	Native vacancy defects in bismuth sulfide. *International Journal of Modern Physics B*, **2014**, 28, 1450150	1.1	10
78	An interplay of sulfur and phosphorus at the □Ni/□-Ni3Al interface. *Journal of Alloys and Compounds*, **2014**, 597, 243-248	5.7	16
77	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	3.9	13
76	Mechanism of Superior Visible-Light Photocatalytic Activity and Stability of Hybrid Ag3PO4/Graphene Nanocomposite. *Journal of Physical Chemistry C*, **2014**, 118, 12972-12979	3.8	71
75	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	5.7	35
74	THE ELECTRONIC AND OPTICAL PROPERTIES OF X-DOPED SrTiO3 (X = Rh, Pd, Ag): A FIRST-PRINCIPLES CALCULATIONS. *International Journal of Modern Physics B*, **2014**, 28, 1450031	1.1	5
73	Negative differential resistance induced by SiNx co-dopant in armchair graphene nanoribbon. *Modern Physics Letters B*, **2014**, 28, 1450229	1.6	3
72	Diverse and tunable electronic structures of single-layer metal phosphorus trichalcogenides for photocatalytic water splitting. *Journal of Chemical Physics*, **2014**, 140, 054707	3.9	76

71	Electronic structures and optical properties of two-dimensional ScN and YN nanosheets. *Journal of Applied Physics*, **2014**, 115, 093504	2.5	23
70	Influence of Pre-Deformation Temperature on Mechanics Performance of NiTiNb Shape Memory Alloy: First-Principles Calculation. *Advanced Materials Research*, **2014**, 1004-1005, 163-167	0.5	
69	Nb solution influencing on phase transformation temperature of Ni47Ti44Nb9 alloy. *Journal of Alloys and Compounds*, **2014**, 609, 156-161	5.7	22
68	First-principles investigation of the binary intermetallics in Mg□Al□r alloy: Stability, elastic properties and electronic structure. *Computational Materials Science*, **2014**, 86, 24-29	3.2	29
67	Band-Gap Widening of Nitrogen-Doped Cu2O: New Insights from First-Principles Calculations. *Science of Advanced Materials*, **2014**, 6, 1221-1227	2.3	9
66	Strain effect on structural and dehydrogenation properties of MgH2 hydride from first-principles calculations. *International Journal of Hydrogen Energy*, **2013**, 38, 3661-3669	6.7	28
65	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	3.9	23
64	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	3.3	9
63	Enhancement of the hole-induced d0-ferromagnetism in ZnO through compensated donor□cceptor complexes: a first-principles study. *Semiconductor Science and Technology*, **2013**, 28, 035017	1.8	8
62	Rectifying behaviors introduced by nitrogen-vacancy complex in spiral chirality single walled carbon nanotube device. *Journal of Applied Physics*, **2013**, 114, 083711	2.5	1
61	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	1.6	7
60	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	3.3	2
59	Kinetic details of crystallization in supercooled liquid Pb during the isothermal relaxation. *Physica B: Condensed Matter*, **2012**, 407, 240-245	2.8	12
58	Microcosmic mechanism of carbon influencing on NiTiNb9 alloy. *Journal of Alloys and Compounds*, **2012**, 542, 170-176	5.7	20
57	Origins of high visible light transparency and solar heat-shielding performance in LaB6. *Applied Physics Letters*, **2012**, 101, 041913	3.4	55
56	Microstructural evolution and martensitic transformation mechanisms during solidification processes of liquid metal Pb. *Philosophical Magazine*, **2012**, 92, 571-585	1.6	7
55	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	5.7	34
54	The correlation between Re and P and their synergetic effect on the rupture strength of the □Ni/□-Ni3Al interface. *Computational Materials Science*, **2012**, 63, 292-302	3.2	15

53	Thermal stability and elastic properties of Mg2X (X = Si, Ge, Sn, Pb) phases from first-principle calculations. *Computational Materials Science*, **2012**, 51, 409-414	3.2	66
52	Structural, elastic and electronic properties of θ(Al2Cu) and S (Al2CuMg) strengthening precipitates in Al–Cu–Mg series alloys: First-principles calculations. *Solid State Communications*, **2012**, 152, 2100-2104	1.6	70
51	Electronic and optical properties of vacancy-doped WS2 monolayers. *AIP Advances*, **2012**, 2, 042141	1.5	33
50	First-principles investigation of H2O adsorption on a BN co-doped nanotube. *Physica Status Solidi (B): Basic Research*, **2012**, 249, 69-73	1.3	2
49	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	3.3	10
48	Ab initio calculations on energetics and electronic structures of cubic Mg3MNi2 (M=Al, Ti, Mn) hydrogen storage alloys. *International Journal of Hydrogen Energy*, **2011**, 36, 14477-14483	6.7	16
47	Research progress in LiBH4 for hydrogen storage: A review. *International Journal of Hydrogen Energy*, **2011**, 36, 14512-14526	6.7	130
46	Electronic and optical properties of the H2O adsorbed the B-N-C nanotubes. *European Physical Journal B*, **2011**, 81, 133-136	1.2	4
45	Study on the electronic structure and the optical performance of YB6 by the first-principles calculations. *AIP Advances*, **2011**, 1, 022140	1.5	9
44	First-principles study on the dehydrogenation properties and mechanism of Al-doped Mg2NiH4. *International Journal of Hydrogen Energy*, **2011**, 36, 5375-5382	6.7	21
43	Solar radiation shielding material for windows TiN studied from first-principles theory. *Applied Physics Letters*, **2011**, 99, 061906	3.4	10
42	A Calculation Study on the Synthesis Routes of Oh-Al13 Cluster. *Advanced Materials Research*, **2011**, 271-273, 586-591	0.5	
41	Optical Characteristics of La-Doped ZnS Thin Films Prepared by Chemical Bath Deposition. *Chinese Physics Letters*, **2011**, 28, 027806	1.8	8
40	Site preference of S-doping and its influence on the properties of a Ni/Ni3Al interface. *Modelling and Simulation in Materials Science and Engineering*, **2011**, 19, 065002	2	13
39	THE EFFECTS OF CO-DOPING OF B AND N ON THE ELECTRONIC TRANSPORT OF SINGLE-WALLED CARBON NANOTUBES. *Modern Physics Letters B*, **2011**, 25, 1211-1218	1.6	2
38	First-principles calculation on the electronic structure and optical properties of laB₆. *Scientia Sinica: Physica, Mechanica Et Astronomica*, **2011**, 41, 58-65	1.5	8
37	Site preference of Ru in NiAl and valence band structure of NiAl containing Ru: First-principles study and photoelectron spectrum. *Philosophical Magazine Letters*, **2010**, 90, 225-232	1	4
36	Valence band structure of the NiAl–Mo alloy from the photoelectron spectrum. *Philosophical Magazine Letters*, **2010**, 90, 299-311	1	

35	Comparison of valence-band structures of NiAl alloy containing Cr and Ti: Photoelectron spectrum and first-principles calculations. *Intermetallics*, **2010**, 18, 1062-1066	3.5	5
34	Molecular dynamic simulations of nanoindentation in aluminum thin film on silicon substrate. *Applied Surface Science*, **2010**, 256, 6284-6290	6.7	74
33	Thermal stability and elastic properties of Mg3Sb2 and Mg3Bi2 phases from first-principles calculations. *Physica B: Condensed Matter*, **2010**, 405, 2863-2868	2.8	45
32	FIRST--PRINCIPLES CALCULATIONS OF STRUCTURAL STABILITIES AND ELASTIC PROPERTIES OF AB2 TYPE INTERMETALLICS IN ZA62 MAGNESIUM ALLOY. *Jinshu Xuebao/Acta Metallurgica Sinica*, **2010**, 2010, 97-103		9
31	Site preference of Re in NiAl and valence band structure of NiAl containing Re: First-principles study and photoelectron spectrum. *Applied Physics Letters*, **2009**, 94, 233104	3.4	9
30	Freezing structures of free silver nanodroplets: A molecular dynamics simulation study. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 1667-1671	2.3	30
29	First-principles investigation of Mg2Ni phase and high/low temperature Mg2NiH4 complex hydrides. *Journal of Physics and Chemistry of Solids*, **2009**, 70, 32-39	3.9	40
28	The preference of synthesis modes and routes of stable Aln+m (n+m≤13) clusters. *Computational Materials Science*, **2009**, 44, 881-887	3.2	10
27	A calculation study on the configuration of Al12C clusters. *Computational Materials Science*, **2009**, 47, 302-307	3.2	2
26	Simulation study of size distributions and magic number sequences of clusters during the solidification process in liquid metal Na. *Journal of Non-Crystalline Solids*, **2009**, 355, 541-547	3.9	12
25	A first-principles study on the structural stability of Al2Ca Al4Ca and Mg2Ca phases. *Materials Letters*, **2008**, 62, 206-210	3.3	41
24	Formation and evolution of metastable bcc phase during solidification of liquid Ag: a molecular dynamics simulation study. *Journal of Physical Chemistry A*, **2008**, 112, 12326-36	2.8	40
23	Molecular dynamics simulation for cooling rate dependence of solidification microstructures of silver. *Journal of Non-Crystalline Solids*, **2008**, 354, 3705-3712	3.9	65
22	Quantum transport properties of carbon nanotube with topologic defects. *EPJ Applied Physics*, **2008**, 43, 19-22	1.1	4
21	Study on H atoms diffusion and adsorption properties of MgH2-V systems. *Science in China Series D: Earth Sciences*, **2008**, 51, 979-988		1
20	Effects of nitrogen substitutional doping on the electronic transport of carbon nanotube. *Physica E: Low-Dimensional Systems and Nanostructures*, **2008**, 40, 462-466	3	37
19	First-principles investigation of Mg2THy (T=Ni, Co, Fe) complex hydrides. *Physica B: Condensed Matter*, **2008**, 403, 4217-4223	2.8	13
18	Effects of nitrogen in Stone-Wales defect on the electronic transport of carbon nanotube. *Applied Physics Letters*, **2007**, 91, 092121	3.4	20

17	Curvature effects on electronic properties of small radius nanotube. *Applied Physics Letters*, **2007**, 91, 033102	3.4	10
16	Formation and magic number characteristics of clusters formed during solidification processes. *Journal of Physics Condensed Matter*, **2007**, 19, 196103	1.8	45
15	Electronic structure and stability of MgTe intermetallic compounds from first-principles calculations. *Journal of Alloys and Compounds*, **2007**, 428, 316-321	5.7	42
14	Structural stability of intermetallic compounds of Mg-Al-Ca alloy. *Transactions of Nonferrous Metals Society of China*, **2007**, 17, 250-256	3.3	23
13	First-principles calculation of dehydrogenating properties of MgH2-V systems. *Science in China Series D: Earth Sciences*, **2006**, 49, 129-136		34
12	Size distributions and magic number characteristics of cluster configurations formed during solidification processes of liquid metal Al. *Science in China Series D: Earth Sciences*, **2006**, 49, 172-187		4
11	Structure stability and configuration evolution of Aln (n=3, 4, 6, 13, 19) clusters. *Science in China Series D: Earth Sciences*, **2006**, 49, 385-392		6
10	First-principles study on structural stability of 3d transition metal alloying magnesium hydride. *Transactions of Nonferrous Metals Society of China*, **2006**, 16, 23-32	3.3	12
9	Configuration evolution of Aln(n=3,4,6,13,19) clusters studied using linear synchronous transit method. *Transactions of Nonferrous Metals Society of China*, **2006**, 16, s808-s812	3.3	5
8	First-principle investigation of bismuth segregation at Σ5 (012) grain-boundaries in nickel. *Transactions of Nonferrous Metals Society of China*, **2006**, 16, s813-s819	3.3	6
7	First-principles study of alloying effect of Re on properties of Ni/Ni3Al interface. *Computational Materials Science*, **2006**, 38, 354-361	3.2	39
6	First-principles study of the properties of Ni/Ni3Al interface doped with B or P. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2006**, 416, 169-175	5.3	27
5	Mechanical alloying and electronic simulations of 2MgFe mixture powders for hydrogen storage. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing* , **2006**, 427, 306-315	5.3	33
4	First principles study of effect of lattice misfit on the bonding strength of Ni/Ni3Al interface. *Journal of Materials Science*, **2004**, 39, 3957-3963	4.3	17
3	The high-temperature properties of microstructure transitions in liquid metal Al. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1999**, 57, 214-217	3.1	12
2	A method for estimating total effective conducting electron numbers of amorphous TM-M alloys with high metalloid content. *Materials Science and Engineering B: Solid-State Materials for Advanced Technology*, **1996**, 41, 258-260	3.1	1
1	Filings Morphology-Dependent Hydrogen Storage Properties of Magnesium-Rich MgNiZn Alloy. *Transactions of the Indian Institute of Metals*,1	1.2	1