

Ping Peng

List of Publications by Year in descending order

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203
papers

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117571

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times ranked

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citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanical properties, thermophysical properties and electronic structure of Yb ³⁺ or Ce ⁴⁺ -doped La ₂ Zr ₂ O ₇ -based TBCs. <i>Journal of Rare Earths</i> , 2023, 41, 588-598.	2.5	2
2	Competition between TCP and crystalline clusters during phase transition of rapidly super-cooled aluminum. <i>Journal of Non-Crystalline Solids</i> , 2022, 576, 121271.	1.5	8
3	First-principles investigations of the fracture toughness of NbCr ₂ alloyed by X (V, Mo, Ti, Fe). <i>Solid State Communications</i> , 2022, 344, 114664.	0.9	1
4	Study on the structural, mechanical, and dynamical stabilities and properties of Nb ₂ AN (A=Si, Ge, and Sn) MAX phases by first principle. <i>Journal of the American Ceramic Society</i> , 2022, 105, 5285-5298.	1.9	4
5	Spinodal limits of supercooled liquid Al deduced from configuration heredity of crystal clusters. <i>Computational Materials Science</i> , 2022, 207, 111316.	1.4	3
6	Cu-induced enhancement of interfacial bonding for brazed diamond grits with Ni Cr filler alloys. <i>International Journal of Refractory Metals and Hard Materials</i> , 2022, 106, 105874.	1.7	8
7	Laser in-situ preparation and mechanical properties of VC reinforced Fe-based wear-resistant composite cladding. <i>Ceramics International</i> , 2022, 48, 28240-28249.	2.3	18
8	Theory-guided construction of electron-deficient sites via removal of lattice oxygen for the boosted electrocatalytic synthesis of ammonia. <i>Nano Research</i> , 2021, 14, 1457-1464.	5.8	10
9	Hydrogen storage properties and mechanisms of as-cast, homogenized and ECAP processed Mg _{98.5} Y ₁ Zn _{0.5} alloys containing LPSO phase. <i>Energy</i> , 2021, 217, 119315.	4.5	22
10	Micromechanism in fracture toughness of NbCr ₂ laves phase improved by nickel alloying: first-principles calculation. <i>Journal of Alloys and Compounds</i> , 2021, 857, 158040.	2.8	8
11	Stabilization of low-valence transition metal towards advanced catalytic effects on the hydrogen storage performance of magnesium hydride. <i>Journal of Magnesium and Alloys</i> , 2021, 9, 647-657.	5.5	53
12	Hydrogen-substituted graphdiyne/graphene as an sp ² /sp ² hybridized carbon interlayer for lithium-sulfur batteries. <i>Nanoscale</i> , 2021, 13, 3817-3826.	2.8	27
13	Insight into the surface activity of defect structure in $\hat{I}\pm$ -MnO ₂ nanorod: first-principles research. <i>Scientific Reports</i> , 2021, 11, 4751.	1.6	0
14	Identification of critical nuclei in the rapid solidification via configuration heredity. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 175701.	0.7	1
15	Effect of intrinsic point-defect complex on elastic properties of $\hat{I}^3\hat{a}^2$ -Ni ₃ Al phases. <i>Materials Research Express</i> , 2021, 8, 066517.	0.8	1
16	Nanometer effect promoting arsenic removal on $\hat{I}\pm$ -MnO ₂ nano-surface in aqueous solution: DFT+U research. <i>Environmental Science and Pollution Research</i> , 2021, 28, 65899-65910.	2.7	1
17	Impact of replacement of Re by W on dislocation slip mediated creeps of $\hat{I}^3\hat{a}^2$ -Ni ₃ Al phases. <i>Transactions of Nonferrous Metals Society of China</i> , 2021, 31, 2013-2023.	1.7	7
18	Effects of Ce and La elements on interfacial bonding, thermal damage and mechanical performance of brazed diamonds with Ni Cr filler alloy. <i>International Journal of Refractory Metals and Hard Materials</i> , 2021, 98, 105571.	1.7	14

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19	Filings Morphology-Dependent Hydrogen Storage Properties of Magnesium-Rich Mg-Y-Zn Alloy. Transactions of the Indian Institute of Metals, 2021, 74, 3171-3184.	0.7	2
20	Doped effect of Gd and Y elements on corrosion resistance of ZrO ₂ in CMAS melt: First-principles and experimental study. Journal of the European Ceramic Society, 2021, 41, 7893-7901.	2.8	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.	1.7	4
22	Effect of Fe doping on structural, elastic and electronic properties of B ₂ ZrCu phase under hydrostatic pressure: A first-principles study. Materials Chemistry and Physics, 2021, 272, 124978.	2.0	3
23	Lowest-energy structural and electronic properties of Cu ₂ Zr ₁₃ (n=3-10) clusters in metallic glasses via CALYPSO search and density functional theory calculations. Journal of Molecular Liquids, 2021, 343, 117603.	2.3	9
24	Impact of Re-clustering on resistances to dislocation slip mediated plastic deformations in β^3 matrix phases. Computational Materials Science, 2020, 172, 109314.	1.4	6
25	Bismuthene from sonoelectrochemistry as a superior anode for potassium-ion batteries. Journal of Materials Chemistry A, 2020, 8, 453-460.	5.2	94
26	Adsorption and diffusion behaviors of Ni-based filler elements on diamond surface. Journal of Alloys and Compounds, 2020, 822, 153652.	2.8	25
27	Different structural transitions of rapidly supercooled tantalum melt under pressure. Physical Chemistry Chemical Physics, 2020, 22, 18078-18090.	1.3	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.	1.4	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.	3.1	10
30	Nearly golden-ratio order in Ta metallic glass*. Chinese Physics B, 2020, 29, 046105.	0.7	4
31	First-principles investigation on electronic structure and solar radiation shielding performance of Ti _{0.33} WO ₃ . Wuli Xuebao/Acta Physica Sinica, 2020, 69, 047102.	0.2	0
32	Monolayer Phosphorene-Carbon Nanotube Heterostructures for Photocatalysis: Analysis by Density Functional Theory. Nanoscale Research Letters, 2019, 14, 233.	3.1	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.	5.4	63
34	Atomic structure insight into crystallization of undercooled liquid metal Zr during isothermal relaxation processes. Philosophical Magazine, 2019, 99, 2904-2919.	0.7	4
35	A synergistic reinforcement of Re and W for ideal shear strengths of β^3 -Ni ₃ Al phases. Journal of Physics and Chemistry of Solids, 2019, 131, 34-43.	1.9	18
36	Wetting mechanism of CMAS melt on YSZ surface at high temperature: First-principles calculation. Applied Surface Science, 2019, 483, 811-818.	3.1	27

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37	The short-range order in liquid and A15 crystal of zirconium. <i>Journal of Non-Crystalline Solids</i> , 2019, 513, 111-119.	1.5	32
38	Enhanced permeability of rGO/S-GO layered membranes with tunable inter-structure for effective rejection of salts and dyes. <i>Separation and Purification Technology</i> , 2019, 220, 309-319.	3.9	51
39	Copper-catalyzed Oxidative C-C ³ -H/N-H Cross-Coupling of Hydrocarbons with P(O)-NH Compounds: the Accelerating Effect Induced by Carboxylic Acid Coproduct. <i>Advanced Synthesis and Catalysis</i> , 2019, 361, 1689-1696.	2.1	1
40	Predictions of electronic structures and optical performance of potential near infrared absorber Sn _{0.33} WO ₃ . <i>AIP Advances</i> , 2019, 9, 115014.	0.6	4
41	Study on the surface activity of t-YSZ nanomaterials by first-principles calculation. <i>Applied Surface Science</i> , 2019, 471, 1072-1082.	3.1	5
42	Novel cellulose-GO/MoS ₂ composites membranes with enhanced permeability for effective salts and dyes rejection at low pressure. <i>Journal of Membrane Science</i> , 2019, 574, 112-123.	4.1	147
43	Reduced Graphene Oxide-Refined Cu Matrix Composites: An Experimental and First-Principles Study. <i>Crystal Research and Technology</i> , 2019, 54, 1800191.	0.6	3
44	Insights Into Interfacial Interaction and Its Influence on the Electronic and Optical Properties of Two-Dimensional WS ₂ /TX ₂ CO ₂ (TX = Ti, Zr) van der Waals Heterostructures. <i>Physica Status Solidi (B): Basic Research</i> , 2019, 256, 1800377.	0.7	2
45	Identification and tracking of different types of crystalline nucleiduring isothermal crystallization of amorphous Ag. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2019, 68, 076401.	0.2	3
46	Electronic structures and optical properties of Ce-doped anatase TiO ₂ with oxygen vacancy. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2019, 68, 037101.	0.2	3
47	Effects of high pressure on microstructure evolution and crystallization mechanisms during solidification of nickel. <i>Materials Research Express</i> , 2018, 5, 036507.	0.8	4
48	Interfacial Interaction between Boron Cluster and Metal Oxide Surface and Its Effects: A Case Study of B ₂₀ /Ag ₃ PO ₄ van der Waals Heterostructure. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6151-6158.	1.5	7
49	Research on the removal mechanism of antimony on $\hat{\pm}$ -MnO ₂ nanorod in aqueous solution: DFT+U method. <i>Journal of Hazardous Materials</i> , 2018, 354, 8-16.	6.5	22
50	Correlation between the chemical order and nature property of Cu-centered Cu-Zr icosahedral clusters. <i>Materials Research Express</i> , 2018, 5, 046302.	0.8	3
51	Derivative effect of laser cladding on interface stability of YSZ@Ni coating on GH4169 alloy: An experimental and theoretical study. <i>Applied Surface Science</i> , 2018, 427, 1105-1113.	3.1	9
52	Arsenic adsorption on $\hat{\pm}$ -MnO ₂ nanofibers and the significance of (1 0 0) facet as compared with (1 1 0). <i>Chemical Engineering Journal</i> , 2018, 331, 492-500.	6.6	106
53	Interfacial Interactions in Monolayer and Few-Layer SnS/CH ₃ NH ₃ PbI ₃ Perovskite van der Waals Heterostructures and Their Effects on Electronic and Optical Properties. <i>ChemPhysChem</i> , 2018, 19, 291-299.	1.0	12
54	Effect of P-Doping on the Rupture Strength of $\hat{\pm}$ -Ni/ $\hat{\pm}$ -Ni ₃ Al Interfaces. <i>IOP Conference Series: Materials Science and Engineering</i> , 2018, 381, 012161.	0.3	2

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55	Theory-Driven Heterojunction Photocatalyst Design with Continuously Adjustable Band Gap Materials. <i>Journal of Physical Chemistry C</i> , 2018, 122, 28065-28074.	1.5	20
56	Cs _{0.33} WO ₃ as a high-performance transparent solar radiation shielding material for windows. <i>Journal of Applied Physics</i> , 2018, 124, .	1.1	14
57	Enhanced hydrogen storage properties and mechanisms of magnesium hydride modified by transition metal dissolved magnesium oxides. <i>International Journal of Hydrogen Energy</i> , 2018, 43, 21864-21873.	3.8	31
58	Evolution of local atomic structures during rapid solidification of liquid metal W. <i>Modern Physics Letters B</i> , 2018, 32, 1850368.	1.0	4
59	In Situ Tuning of Catalytic Activity by Thermoelectric Effect for Ethylene Oxidation. <i>ACS Catalysis</i> , 2018, 8, 10164-10172.	5.5	20
60	Impact of correlative defects induced by double Re-addition on the ideal shear strength of $\hat{\Gamma}$ -Ni ₃ Al phases. <i>Computational Materials Science</i> , 2018, 152, 408-416.	1.4	19
61	Evolution Mechanism of Metallic Dioxide MO ₂ (M = Mn, Ti) from Nanorods to Bulk Crystal: First-Principles Research. <i>Journal of Nanomaterials</i> , 2018, 2018, 1-14.	1.5	3
62	Mechanism of crack nucleation and growth in YSZ thermal barrier coatings corroded by CMAS at high temperatures: First-principles calculation. <i>Corrosion Science</i> , 2018, 142, 258-265.	3.0	25
63	Simultaneous dispersive and covalent monolayer MoS ₂ /TiO ₂ cluster heterostructures: Insights into their enhanced photocatalytic activity. <i>Superlattices and Microstructures</i> , 2018, 121, 64-74.	1.4	0
64	Local atomic structures of amorphous Pd ₈₀ Si ₂₀ alloys and their configuration heredity in the rapid solidification. <i>Philosophical Magazine</i> , 2018, 98, 2861-2877.	0.7	9
65	Correlation between the chemical short-range order and binding energy of Cu-centred Cu _n Zr ₁₃ (n=6,7,8,9) icosahedral clusters in metallic glass. <i>Molecular Simulation</i> , 2018, 44, 1183-1190.	0.9	4
66	Tuning the near-gap electronic structure of Cu ₂ O by anion-cation co-doping for enhanced solar energy conversion. <i>Modern Physics Letters B</i> , 2017, 31, 1650429.	1.0	4
67	Electronic and optical properties of Cr-, B-doped, and (Cr, B)-codoped SrTiO ₃ . <i>International Journal of Modern Physics B</i> , 2017, 31, 1750064.	1.0	2
68	A DFT study on the competition and evolution characteristics between icosahedra and FCC clusters in rapid solidification of liquid Ag. <i>Journal of Molecular Liquids</i> , 2017, 230, 271-279.	2.3	7
69	Simultaneous covalent and noncovalent carbon nanotube/Ag ₃ PO ₄ hybrids: new insights into the origin of enhanced visible light photocatalytic performance. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 7955-7963.	1.3	13
70	High-temperature oxidation resistance of the Ni ₆₀ Ti alloy: An experimental and first-principles study. <i>Journal of Alloys and Compounds</i> , 2017, 706, 297-304.	2.8	9
71	Hybrid TiO ₂ /graphene derivatives nanocomposites: is functionalized graphene better than pristine graphene for enhanced photocatalytic activity?. <i>Catalysis Science and Technology</i> , 2017, 7, 1423-1432.	2.1	20
72	Antimony Removal from Aqueous Solution Using Novel $\hat{\Gamma}$ -MnO ₂ Nanofibers: Equilibrium, Kinetic, and Density Functional Theory Studies. <i>ACS Sustainable Chemistry and Engineering</i> , 2017, 5, 2255-2264.	3.2	85

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73	Structural evolutions and hereditary characteristics of icosahedral nano-clusters formed in Mg ₇₀ Zn ₃₀ alloys during rapid solidification processes. <i>Scientific Reports</i> , 2017, 7, 43111.	1.6	11
74	Alkali metal silanides $\sqrt{3}$ -MSiH ₃ : A family of complex hydrides for solid-state hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 12405-12413.	3.8	15
75	Effects of pressure on microstructure evolution and mechanical properties of liquid Ni ₆₄ Zr ₃₆ alloy during rapid solidification: A molecular dynamics simulation study. <i>Computational Materials Science</i> , 2017, 137, 30-38.	1.4	8
76	Effect of high pressure on the formation and evolution of clusters during the rapid solidification of zirconium melts. <i>Computational Materials Science</i> , 2017, 140, 275-283.	1.4	21
77	Noncovalent Functionalization of Monolayer MoS ₂ with Carbon Nanotubes: Tuning Electronic Structure and Photocatalytic Activity. <i>Journal of Physical Chemistry C</i> , 2017, 121, 21921-21929.	1.5	23
78	High-temperature corrosion mechanism of YSZ coatings subject to calcium-magnesium-aluminosilicate (CMAS) deposits: First-principles calculations. <i>Corrosion Science</i> , 2017, 126, 286-294.	3.0	47
79	The mechanism of enhanced photocatalytic activity of SnO ₂ through fullerene modification. <i>Current Applied Physics</i> , 2017, 17, 1547-1556.	1.1	14
80	First-principles study of electronic, mechanical and optical properties of mixed valence SmB ₆ . <i>IOP Conference Series: Materials Science and Engineering</i> , 2017, 207, 012084.	0.3	3
81	Mechanism of surface effect and selective catalytic performance of MnO ₂ nanorod: DFT+U study. <i>Applied Surface Science</i> , 2017, 420, 205-213.	3.1	19
82	Enhanced hydrogen diffusion in magnesium based hydride induced by strain and doping from first principle study. <i>Journal of Alloys and Compounds</i> , 2017, 694, 687-693.	2.8	18
83	A comparative study on local atomic configurations characterized by cluster-type-index method and Voronoi polyhedron method. <i>Computational Materials Science</i> , 2016, 123, 214-223.	1.4	35
84	First-principles investigation on solar radiation shielding performance of rutile VO ₂ filters for smart windows. <i>Applied Physics Letters</i> , 2016, 109, .	1.5	10
85	First-principles prediction of solar radiation shielding performance for transparent windows of GdB ₆ . <i>Journal of Applied Physics</i> , 2016, 119, .	1.1	14
86	Dual role of monolayer MoS ₂ in enhanced photocatalytic performance of hybrid MoS ₂ /SnO ₂ nanocomposite. <i>Journal of Applied Physics</i> , 2016, 119, .	1.1	57
87	Near-infrared radiation absorption properties of covellite (CuS) using first-principles calculations. <i>AIP Advances</i> , 2016, 6, .	0.6	21
88	Investigation on the electronic structures and optical performances of S-codoped anatase TiO ₂ by first-principles calculation. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 1462-1468.	0.9	10
89	Solar radiation shielding properties of transparent LaB ₆ filters through experimental and first-principles calculation methods. <i>Ceramics International</i> , 2016, 42, 14278-14281.	2.3	15
90	Electronic properties and photoactivity of monolayer MoS ₂ /fullerene van der Waals heterostructures. <i>RSC Advances</i> , 2016, 6, 43228-43236.	1.7	28

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91	Non-covalent functionalization of WS ₂ monolayer with small fullerenes: tuning electronic properties and photoactivity. Dalton Transactions, 2016, 45, 13383-13391.	1.6	22
92	Dual functions of 2D WS ₂ and MoS ₂ as WS ₂ monolayers coupled with a Ag ₃ PO ₄ photocatalyst. Semiconductor Science and Technology, 2016, 31, 095013.	1.0	8
93	Predictions of solar radiation shielding properties of KB 6 from first principles. Computational Condensed Matter, 2016, 9, 1-5.	0.9	4
94	Molecular dynamics study on microstructural evolution during crystallization of rapidly supercooled zirconium melts. Journal of Alloys and Compounds, 2016, 688, 654-665.	2.8	38
95	Effective interactions and atomic ordering in Ni-rich Ni-Re alloys. Physical Review B, 2016, 94, .	1.1	19
96	Dramatically Enhanced Visible Light Response of Monolayer ZrS ₂ via Non-covalent Modification by Double-Ring Tubular B ₂₀ Cluster. Nanoscale Research Letters, 2016, 11, 495.	3.1	25
97	Tuning near-gap electronic structure, interface charge transfer and visible light response of hybrid doped graphene and Ag ₃ PO ₄ composite: Dopant effects. Scientific Reports, 2016, 6, 22267.	1.6	24
98	Crystallization characteristics in supercooled liquid zinc during isothermal relaxation: A molecular dynamics simulation study. Scientific Reports, 2016, 6, 31653.	1.6	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.	10.8	23
100	Enhanced photocatalytic performance of an Ag ₃ PO ₄ photocatalyst via fullerene modification: first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 2878-2886.	1.3	22
101	Structural stability of characteristic interface for NiTi/Nb Nanowire: First-Principle study. Metals and Materials International, 2016, 22, 69-74.	1.8	5
102	Cohesive mechanism of the FeCr/Ni Interface: A first-principles study. Metals and Materials International, 2016, 22, 75-80.	1.8	5
103	Strain tuned dehydrogenation thermodynamics of magnesium based hydride: A first principle study. Computational Materials Science, 2015, 105, 71-74.	1.4	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.	0.3	4
105	Effects of S/Ce-codoping on electronic structures and optical properties of anatase TiO ₂ from density functional theory calculations. Modern Physics Letters B, 2015, 29, 1550249.	1.0	1
106	Effect of cooling rates on clustering towards icosahedra in rapidly solidified Cu ₅₆ Zr ₄₄ alloy. Transactions of Nonferrous Metals Society of China, 2015, 25, 533-543.	1.7	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.	1.9	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.	1.4	13

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109	Electronic Structures and Photocatalytic Responses of SrTiO ₃ (100) Surface Interfaced with Graphene, Reduced Graphene Oxide, and Graphane: Surface Termination Effect. Journal of Physical Chemistry C, 2015, 119, 19095-19104.	1.5	32
110	Phase stability, elastic properties and electronic structures of Mg-Y intermetallics from first-principles calculations. Journal of Magnesium and Alloys, 2015, 3, 127-133.	5.5	27
111	Enhancement of transport properties introduced complex defect in (6, 3) carbon nanotubes. Modern Physics Letters B, 2015, 29, 1550031.	1.0	0
112	Non-linear effects of initial melt temperatures on microstructures and mechanical properties during quenching process of liquid Cu ₄₆ Zr ₅₄ alloy. Physica B: Condensed Matter, 2015, 465, 81-88.	1.3	4
113	Optical transportation and controllable positioning of nanospheres using a microfiber. AIP Advances, 2015, 5, .	0.6	5
114	Correlation of the heredity of icosahedral clusters with the glass forming ability of rapidly solidified Cu x Zr 100 ^x alloys. Journal of Non-Crystalline Solids, 2015, 427, 199-207.	1.5	24
115	Band structure engineering of monolayer MoS ₂ : a charge compensated codoping strategy. RSC Advances, 2015, 5, 7944-7952.	1.7	26
116	Dehydrogenation thermodynamics of magnesium hydride doped with transition metals: Experimental and theoretical studies. Computational Materials Science, 2015, 98, 211-219.	1.4	32
117	Magnetic properties of Ni-doped ZnS: First-principles study. Journal of Magnetism and Magnetic Materials, 2015, 377, 239-242.	1.0	21
118	Formation and evolution of nano-clusters in a large-scale system of Cu-Zr alloy during rapid solidification process. Computational Materials Science, 2015, 98, 1-9.	1.4	15
119	THE ELECTRONIC AND OPTICAL PROPERTIES OF X-DOPED SrTiO ₃ (X = Rh, Pd, Tj) 1.0 ± 0.784314 rgBT	1.0	8
120	Negative differential resistance induced by SiN _x co-dopant in armchair graphene nanoribbon. Modern Physics Letters B, 2014, 28, 1450229.	1.0	3
121	Diverse and tunable electronic structures of single-layer metal phosphorus trichalcogenides for photocatalytic water splitting. Journal of Chemical Physics, 2014, 140, 054707.	1.2	99
122	Electronic structures and optical properties of two-dimensional ScN and YN nanosheets. Journal of Applied Physics, 2014, 115, .	1.1	30
123	Nb solution influencing on phase transformation temperature of Ni ₄₇ Ti ₄₄ Nb ₉ alloy. Journal of Alloys and Compounds, 2014, 609, 156-161.	2.8	24
124	First-principles investigation of the binary intermetallics in Mg-Al-Sr alloy: Stability, elastic properties and electronic structure. Computational Materials Science, 2014, 86, 24-29.	1.4	36
125	Band engineering of ZnS by codoping for visible-light photocatalysis. Applied Physics A: Materials Science and Processing, 2014, 116, 741-750.	1.1	32
126	Band gap engineering by lanthanide doping in the photocatalyst LaOF: First-principles study. International Journal of Modern Physics B, 2014, 28, 1450069.	1.0	6

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127	Single-layer Group-IVB nitride halides as promising photocatalysts. Journal of Materials Chemistry A, 2014, 2, 6755.	5.2	90
128	Native vacancy defects in bismuth sulfide. International Journal of Modern Physics B, 2014, 28, 1450150.	1.0	15
129	An interplay of sulfur and phosphorus at the $\text{Ni}_3\text{-Ni}_3\text{Al}$ interface. Journal of Alloys and Compounds, 2014, 597, 243-248.	2.8	21
130	The effect of cooling rates on hereditary characteristics of icosahedral clusters in rapid solidification of liquid Cu ₅₆ Zr ₄₄ alloys. Journal of Non-Crystalline Solids, 2014, 388, 75-85.	1.5	16
131	Mechanism of Superior Visible-Light Photocatalytic Activity and Stability of Hybrid Ag ₃ PO ₄ /Graphene Nanocomposite. Journal of Physical Chemistry C, 2014, 118, 12972-12979.	1.5	78
132	Influence of icosahedral order on the second peak splitting of pair distribution function for Mg ₇₀ Zn ₃₀ metallic glass. Journal of Alloys and Compounds, 2014, 597, 269-274.	2.8	45
133	Band-Gap Widening of Nitrogen-Doped Cu ₂ O: New Insights from First-Principles Calculations. Science of Advanced Materials, 2014, 6, 1221-1227.	0.1	10
134	Strain effect on structural and dehydrogenation properties of MgH ₂ hydride from first-principles calculations. International Journal of Hydrogen Energy, 2013, 38, 3661-3669.	3.8	41
135	On the heredity and evolution of icosahedral clusters during the rapid solidification of liquid Cu ₅₀ Zr ₅₀ alloys. Journal of Non-Crystalline Solids, 2013, 378, 61-70.	1.5	27
136	Simulation study on non-linear effects of initial melt temperatures on microstructures during solidification process of liquid Mg ₇ Zn ₃ alloy. Transactions of Nonferrous Metals Society of China, 2013, 23, 1052-1060.	1.7	10
137	Enhancement of the hole-induced d ⁰ -ferromagnetism in ZnO through compensated donor-acceptor complexes: a first-principles study. Semiconductor Science and Technology, 2013, 28, 035017.	1.0	8
138	Rectifying behaviors introduced by nitrogen-vacancy complex in spiral chirality single walled carbon nanotube device. Journal of Applied Physics, 2013, 114, .	1.1	1
139	TUNING THE "d ⁰ " FERROMAGNETISM IN In_2O_3 QUANTUM DOTS BY DANGLING BONDS AND VACANCY BASED ON THE FIRST-PRINCIPLE CALCULATION. Modern Physics Letters B, 2013, 27, 1350068.	1.0	7
140	Optical and Electronic Properties of Ni-Doped ZnS: First-Principles Study. Journal of Nanoelectronics and Optoelectronics, 2013, 8, 297-301.	0.1	1
141	A TS Search for Stable Configurations of Double Icosahedral Ag _n (n=19, 23, 24, 25) Clusters Linked by Sharing Atoms. Acta Chimica Sinica, 2013, 71, 1429.	0.5	3
142	Microcosmic mechanism of carbon influencing on NiTiNb ₉ alloy. Journal of Alloys and Compounds, 2012, 542, 170-176.	2.8	22
143	Origins of high visible light transparency and solar heat-shielding performance in LaB ₆ . Applied Physics Letters, 2012, 101, 041913.	1.5	62
144	Microstructural evolution and martensitic transformation mechanisms during solidification processes of liquid metal Pb. Philosophical Magazine, 2012, 92, 571-585.	0.7	10

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145	Synergistic effect of Ti and F co-doping on dehydrogenation properties of MgH ₂ from first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2012, 538, 205-211.	2.8	35
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