# Ping Peng

List of Publications by Year
in descending order

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Version: 2024-02-01

| 203 | 4,195 | 117619 | 175241 |
|---|---|---|---|
| papers | citations | 34 h-index | 52 g-index |

| 203 | 203 | 203 | 4504 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Research progress in LiBH4 for hydrogen storage: A review. International Journal of Hydrogen Energy, 2011, 36, 14512-14526. | 7.1 | 154 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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 |
| 5 | 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 |
| 6 | Molecular dynamic simulations of nanoindentation in aluminum thin film on silicon substrate. Applied Surface Science, 2010, 256, 6284-6290. | 6.1 | 96 |
| 7 | Bismuthene from sonoelectrochemistry as a superior anode for potassium-ion batteries. Journal of Materials Chemistry A, 2020, 8, 453-460. | 10.3 | 94 |
| 8 | Single-layer Group-IVB nitride halides as promising photocatalysts. Journal of Materials Chemistry A, 2014, 2, 6755. | 10.3 | 90 |
| 9 | 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 |
| 10 | Antimony Removal from Aqueous Solution Using Novel Î±-MnO<sub>2</sub> Nanofibers: Equilibrium, Kinetic, and Density Functional Theory Studies. ACS Sustainable Chemistry and Engineering, 2017, 5, 2255-2264. | 6.7 | 85 |
| 11 | Mechanism of Superior Visible-Light Photocatalytic Activity and Stability of Hybrid Ag<sub>3</sub>PO<sub>4</sub>/Graphene Nanocomposite. Journal of Physical Chemistry C, 2014, 118, 12972-12979. | 3.1 | 78 |
| 12 | Molecular dynamics simulation for cooling rate dependence of solidification microstructures of silver. Journal of Non-Crystalline Solids, 2008, 354, 3705-3712. | 3.1 | 75 |
| 13 | 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 |
| 14 | Origins of high visible light transparency and solar heat-shielding performance in LaB<sub>6</sub>. Applied Physics Letters, 2012, 101, 041913. | 3.3 | 62 |
| 15 | Thermal stability and elastic properties of Mg3Sb2 and Mg3Bi2 phases from first-principles calculations. Physica B: Condensed Matter, 2010, 405, 2863-2868. | 2.7 | 60 |
| 16 | Dual role of monolayer MoS2 in enhanced photocatalytic performance of hybrid MoS2/SnO2 nanocomposite. Journal of Applied Physics, 2016, 119, . | 2.5 | 57 |
| 17 | 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 |
| 18 | First-principles investigation of Mg2Ni phase and high/low temperature Mg2NiH4 complex hydrides. Journal of Physics and Chemistry of Solids, 2009, 70, 32-39. | 4.0 | 51 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | A first-principles study on the structural stability of Al2Ca Al4Ca and Mg2Ca phases. Materials Letters, 2008, 62, 206-210. | 2.6 | 50 |
| 21 | Formation and magic number characteristics of clusters formed during solidification processes. Journal of Physics Condensed Matter, 2007, 19, 196103. | 1.8 | 49 |
| 22 | 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 |
| 23 | Electronic structure and stability of Mgâ€“Ce intermetallic compounds from first-principles calculations. Journal of Alloys and Compounds, 2007, 428, 316-321. | 5.5 | 45 |
| 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, 12326-12336. | 2.5 | 45 |
| 25 | 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 |
| 26 | First-principles study of alloying effect of Re on properties of Ni/Ni3Al interface. Computational Materials Science, 2006, 38, 354-361. | 3.0 | 42 |
| 27 | First-principles calculation of dehydrogenating properties of MgH2-V systems. Science in China Series D: Earth Sciences, 2006, 49, 129-136. | 0.9 | 42 |
| 28 | Electronic and optical properties of vacancy-doped WS2 monolayers. AIP Advances, 2012, 2, . | 1.3 | 41 |
| 29 | 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 |
| 30 | Effects of nitrogen substitutional doping on the electronic transport of carbon nanotube. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 462-466. | 2.7 | 40 |
| 31 | Mechanical alloying and electronic simulations of 2Mgâ€“Fe mixture powders for hydrogen storage. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2006, 427, 306-315. | 5.6 | 38 |
| 32 | 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 |
| 33 | 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 |
| 34 | 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 |
| 35 | 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 |
| 36 | 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. | 5.6 | 33 |

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| 37 | 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. | 2.1 | 33 |
| 38 | Band engineering of ZnS by codoping for visible-light photocatalysis. Applied Physics A: Materials Science and Processing, 2014, 116, 741-750. | 2.3 | 32 |
| 39 | Electronic Structures and Photocatalytic Responses of SrTiO<sub>3</sub>(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 |
| 40 | Dehydrogenation thermodynamics of magnesium hydride doped with transition metals: Experimental and theoretical studies. Computational Materials Science, 2015, 98, 211-219. | 3.0 | 32 |
| 41 | The short-range order in liquid and A15 crystal of zirconium. Journal of Non-Crystalline Solids, 2019, 513, 111-119. | 3.1 | 32 |
| 42 | 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 |
| 43 | Electronic structures and optical properties of two-dimensional ScN and YN nanosheets. Journal of Applied Physics, 2014, 115, . | 2.5 | 30 |
| 44 | Electronic properties and photoactivity of monolayer MoS<sub>2</sub>/fullerene van der Waals heterostructures. RSC Advances, 2016, 6, 43228-43236. | 3.6 | 28 |
| 45 | 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 |
| 46 | 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 |
| 47 | Wetting mechanism of CMAS melt on YSZ surface at high temperature: First-principles calculation. Applied Surface Science, 2019, 483, 811-818. | 6.1 | 27 |
| 48 | Hydrogen-substituted graphdiyne/graphene as an sp/sp<sup>2</sup> hybridized carbon interlayer for lithiumâ€“sulfur batteries. Nanoscale, 2021, 13, 3817-3826. | 5.6 | 27 |
| 49 | Band structure engineering of monolayer MoS<sub>2</sub>: a charge compensated codoping strategy. RSC Advances, 2015, 5, 7944-7952. | 3.6 | 26 |
| 50 | Structural stability of intermetallic compounds of Mg-Al-Ca alloy. Transactions of Nonferrous Metals Society of China, 2007, 17, 250-256. | 4.2 | 25 |
| 51 | 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 |
| 52 | 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 |
| 53 | Adsorption and diffusion behaviors of Ni-based filler elements on diamond surface. Journal of Alloys and Compounds, 2020, 822, 153652. | 5.5 | 25 |
| 54 | First-principles study on the dehydrogenation properties and mechanism of Al-doped Mg2NiH4. International Journal of Hydrogen Energy, 2011, 36, 5375-5382. | 7.1 | 24 |

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| 55 | Nb solution influencing on phase transformation temperature of Ni47Ti44Nb9 alloy. Journal of Alloys and Compounds, 2014, 609, 156-161. | 5.5 | 24 |
| 56 | 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 |
| 57 | 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 |
| 58 | 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 |
| 59 | Noncovalent Functionalization of Monolayer MoS<sub>2</sub> with Carbon Nanotubes: Tuning Electronic Structure and Photocatalytic Activity. Journal of Physical Chemistry C, 2017, 121, 21921-21929. | 3.1 | 23 |
| 60 | First principles study of effect of lattice misfit on the bonding strength of Ni/Ni<sub>3</sub>Al interface. Journal of Materials Science, 2004, 39, 3957-3963. | 3.7 | 22 |
| 61 | Microcosmic mechanism of carbon influencing on NiTiNb9 alloy. Journal of Alloys and Compounds, 2012, 542, 170-176. | 5.5 | 22 |
| 62 | Non-covalent functionalization of WS<sub>2</sub> monolayer with small fullerenes: tuning electronic properties and photoactivity. Dalton Transactions, 2016, 45, 13383-13391. | 3.3 | 22 |
| 63 | Enhanced photocatalytic performance of an Ag<sub>3</sub>PO<sub>4</sub> photocatalyst via fullerene modification: first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 2878-2886. | 2.8 | 22 |
| 64 | 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 |
| 65 | 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 |
| 66 | 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 |
| 67 | 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 |
| 68 | Magnetic properties of NI-doped ZnS: First-principles study. Journal of Magnetism and Magnetic Materials, 2015, 377, 239-242. | 2.3 | 21 |
| 69 | Near-infrared radiation absorption properties of covellite (CuS) using first-principles calculations. AIP Advances, 2016, 6, . | 1.3 | 21 |
| 70 | 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 |
| 71 | Effects of nitrogen in Stone-Wales defect on the electronic transport of carbon nanotube. Applied Physics Letters, 2007, 91, . | 3.3 | 20 |
| 72 | Hybrid TiO<sub>2</sub>/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 |

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| 73 | Theory-Driven Heterojunction Photocatalyst Design with Continuously Adjustable Band Gap Materials. Journal of Physical Chemistry C, 2018, 122, 28065-28074. | 3.1 | 20 |
| 74 | In Situ Tuning of Catalytic Activity by Thermoelectric Effect for Ethylene Oxidation. ACS Catalysis, 2018, 8, 10164-10172. | 11.2 | 20 |
| 75 | 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 |
| 76 | Effective interactions and atomic ordering in Ni-rich Ni-Re alloys. Physical Review B, 2016, 94, . | 3.2 | 19 |
| 77 | 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 |
| 78 | 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 |
| 79 | 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 |
| 80 | 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 |
| 81 | 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 |
| 82 | 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. | 3.1 | 17 |
| 83 | 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. | 3.5 | 16 |
| 84 | 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 |
| 85 | First-principles investigation of Mg2THy (T=Ni, Co, Fe) complex hydrides. Physica B: Condensed Matter, 2008, 403, 4217-4223. | 2.7 | 15 |
| 86 | Site preference of S-doping and its influence on the properties of a Ni/Ni<sub>3</sub>Al interface. Modelling and Simulation in Materials Science and Engineering, 2011, 19, 065002. | 2.0 | 15 |
| 87 | Native vacancy defects in bismuth sulfide. International Journal of Modern Physics B, 2014, 28, 1450150. | 2.0 | 15 |
| 88 | 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 |
| 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 | Crystallization characteristics in supercooled liquid zinc during isothermal relaxation: A molecular dynamics simulation study. Scientific Reports, 2016, 6, 31653. | 3.3 | 15 |

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| 91 | 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 |
| 92 | First-principles prediction of solar radiation shielding performance for transparent windows of GdB6. Journal of Applied Physics, 2016, 119, . | 2.5 | 14 |
| 93 | The mechanism of enhanced photocatalytic activity of SnO 2 through fullerene modification. Current Applied Physics, 2017, 17, 1547-1556. | 2.4 | 14 |
| 94 | Cs0.33WO3 as a high-performance transparent solar radiation shielding material for windows. Journal of Applied Physics, 2018, 124, . | 2.5 | 14 |
| 95 | 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 |
| 96 | Curvature effects on electronic properties of small radius nanotube. Applied Physics Letters, 2007, 91, . | 3.3 | 13 |
| 97 | Kinetic details of crystallization in supercooled liquid Pb during the isothermal relaxation. Physica B: Condensed Matter, 2012, 407, 240-245. | 2.7 | 13 |
| 98 | 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 |
| 99 | Simultaneous covalent and noncovalent carbon nanotube/Ag<sub>3</sub>PO<sub>4</sub> hybrids: new insights into the origin of enhanced visible light photocatalytic performance. Physical Chemistry Chemical Physics, 2017, 19, 7955-7963. | 2.8 | 13 |
| 100 | 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 |
| 101 | First-principles study on structural stability of 3d transition metal alloying magnesium hydride. Transactions of Nonferrous Metals Society of China, 2006, 16, 23-32. | 4.2 | 12 |
| 102 | Study on the electronic structure and the optical performance of YB6 by the first-principles calculations. AIP Advances, 2011, 1, . | 1.3 | 12 |
| 103 | Interfacial Interactions in Monolayer and Fewâ€Layer SnS/CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> Perovskite van der Waals Heterostructures and Their Effects on Electronic and Optical Properties. ChemPhysChem, 2018, 19, 291-299. | 2.1 | 12 |
| 104 | Optical Characteristics of La-Doped ZnS Thin Films Prepared by Chemical Bath Deposition. Chinese Physics Letters, 2011, 28, 027806. | 3.3 | 11 |
| 105 | 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 |
| 106 | The preference of synthesis modes and routes of stable Aln+m (n+mâ‰13) clusters. Computational Materials Science, 2009, 44, 881-887. | 3.0 | 10 |
| 107 | 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 |
| 108 | Solar radiation shielding material for windows TiN studied from first-principles theory. Applied Physics Letters, 2011, 99, 061906. | 3.3 | 10 |

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| 109 | Microstructural evolution and martensitic transformation mechanisms during solidification processes of liquid metal Pb. Philosophical Magazine, 2012, 92, 571-585. | 1.6 | 10 |
| 110 | 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 |
| 111 | First-principles investigation on solar radiation shielding performance of rutile VO2 filters for smart windows. Applied Physics Letters, 2016, 109, . | 3.3 | 10 |
| 112 | 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 |
| 113 | Monolayer Phosphoreneâ€“Carbon Nanotube Heterostructures for Photocatalysis: Analysis by Density Functional Theory. Nanoscale Research Letters, 2019, 14, 233. | 5.7 | 10 |
| 114 | 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 |
| 115 | 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 |
| 116 | Band-Gap Widening of Nitrogen-Doped Cu<SUB>2</SUB>O: New Insights from First-Principles Calculations. Science of Advanced Materials, 2014, 6, 1221-1227. | 0.7 | 10 |
| 117 | FIRST–PRINCIPLES CALCULATIONS OF STRUCTURAL STABILITIES AND ELASTIC PROPERTIES OF <I>AB</I><SUB>2</SUB> TYPE INTERMETALLICS IN ZA62 MAGNESIUM ALLOY. Jinshu Xuebao/Acta Metallurgica Sinica, 2010, 2010, 97-103. | 0.3 | 10 |
| 118 | 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. | 3.3 | 9 |
| 119 | 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 |
| 120 | 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 |
| 121 | Local atomic structures of amorphous Pd<sub>80</sub>Si<sub>20</sub> alloys and their configuration heredity in the rapid solidification. Philosophical Magazine, 2018, 98, 2861-2877. | 1.6 | 9 |
| 122 | Different structural transitions of rapidly supercooled tantalum melt under pressure. Physical Chemistry Chemical Physics, 2020, 22, 18078-18090. | 2.8 | 9 |
| 123 | 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 |
| 124 | Enhancement of the hole-induced d<sup>0</sup>-ferromagnetism in ZnO through compensated donorâ€“acceptor complexes: a first-principles study. Semiconductor Science and Technology, 2013, 28, 035017. | 2.0 | 8 |
| 125 | THE ELECTRONIC AND OPTICAL PROPERTIES OF X-DOPED <font>SrTiO</font><sub>3</sub> (X = Rh, Pd,) Tj ETQq1 1 0.784314 rgBT | 2.0 | 8 |
| 126 | Strain tuned dehydrogenation thermodynamics of magnesium based hydride: A first principle study. Computational Materials Science, 2015, 105, 71-74. | 3.0 | 8 |

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| 127 | 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 |
| 128 | Dual functions of 2D WS<sub>2</sub>and MoS<sub>2</sub>â€“WS<sub>2</sub>monolayers coupled with a Ag<sub>3</sub>PO<sub>4</sub>photocatalyst. Semiconductor Science and Technology, 2016, 31, 095013. | 2.0 | 8 |
| 129 | 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 |
| 130 | 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 |
| 131 | First-principles calculation on the electronic structure and optical properties of laB<sub>6</sub>. Scientia Sinica: Physica, Mechanica Et Astronomica, 2011, 41, 58-65. | 0.4 | 8 |
| 132 | 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 |
| 133 | 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 |
| 134 | TUNING THE "d<sup>0</sup>" FERROMAGNETISM IN <font>In</font><sub>2</sub><font>O</font><sub>3</sub> QUANTUM DOTS BY DANGLING BONDS AND VACANCY BASED ON THE FIRST-PRINCIPLE CALCULATION. Modern Physics Letters B, 2013, 27, 1350068. | 1.9 | 7 |
| 135 | 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 |
| 136 | Interfacial Interaction between Boron Cluster and Metal Oxide Surface and Its Effects: A Case Study of B<sub>20</sub>/Ag<sub>3</sub>PO<sub>4</sub> van der Waals Heterostructure. Journal of Physical Chemistry C, 2018, 122, 6151-6158. | 3.1 | 7 |
| 137 | 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 |
| 138 | First-principle investigation of bismuth segregation at Î£5 (012) grain-boundaries in nickel. Transactions of Nonferrous Metals Society of China, 2006, 16, s813-s819. | 4.2 | 6 |
| 139 | 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. | 0.9 | 6 |
| 140 | Comparison of valence-band structures of NiAl alloy containing Cr and Ti: Photoelectron spectrum and first-principles calculations. Intermetallics, 2010, 18, 1062-1066. | 3.9 | 6 |
| 141 | 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 |
| 142 | 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 |
| 143 | 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 |
| 144 | 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. | 4.2 | 5 |

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| 145 | 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. | 1.2 | 5 |
| 146 | Optical transportation and controllable positioning of nanospheres using a microfiber. AIP Advances, 2015, 5, . | 1.3 | 5 |
| 147 | Structural stability of characteristic interface for NiTi/Nb Nanowire: First-Principle study. Metals and Materials International, 2016, 22, 69-74. | 3.4 | 5 |
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