Yonghua Duan

List of Publications by Citations

89 papers	1,439 citations	21 h-index	34 g-index
97 ext. papers	2,018 ext. citations	3.3 avg, IF	5.51 L-index

#	Paper	IF	Citations
89	Anisotropic elastic properties of the CaPb compounds. *Journal of Alloys and Compounds*, **2014**, 595, 14-21	5.7	105
88	Phase stability, structural and elastic properties of C15-type Laves transition-metal compounds MCo2 from first-principles calculations. *Journal of Alloys and Compounds*, **2015**, 630, 202-208	5.7	85
87	Stability, elastic properties and electronic structures of the stable ZrAl intermetallic compounds: A first-principles investigation. *Journal of Alloys and Compounds*, **2014**, 590, 50-60	5.7	80
86	Electronic structures, mechanical and thermodynamic properties of cubic alkaline-earth hexaborides from first principles calculations. *Journal of Alloys and Compounds*, **2015**, 635, 213-224	5.7	68
85	Electronic structure, elastic anisotropy, thermal conductivity and optical properties of calcium apatite Ca5(PO4)3X (X = F, Cl or Br). *Journal of Alloys and Compounds*, **2015**, 619, 66-77	5.7	64
84	Structural, anisotropic elastic and thermal properties of MB (M=Ti, Zr and Hf) monoborides. *Ceramics International*, **2015**, 41, 6831-6843	5.1	62
83	A first-principles prediction of anisotropic elasticity and thermal properties of potential superhard WB3. *Ceramics International*, **2018**, 44, 14053-14062	5.1	52
82	Structural properties, elastic anisotropies and thermal conductivities of tetragonal LnB2C2 (Ln = Rare Earth) compounds from first-principles calculations. *Ceramics International*, **2019**, 45, 1857-1867	5.1	42
81	Structural properties, electronic structures and optical properties of WB2 with different structures: A theoretical investigation. *Ceramics International*, **2018**, 44, 11438-11447	5.1	40
80	Developed constitutive models, processing maps and microstructural evolution of Pb-Mg-10Al-0.5B alloy. *Materials Characterization*, **2017**, 129, 353-366	3.9	37
79	Elastic anisotropies and thermal conductivities of WB2 diborides in different crystal structures: A first-principles calculation. *Journal of Alloys and Compounds*, **2018**, 747, 905-915	5.7	37
78	Ab-initio investigations on elastic properties in L12 structure Al3Sc and Al3Y under high pressure. *Journal of Alloys and Compounds*, **2014**, 585, 587-593	5.7	36
77	Thermodynamic properties and thermal conductivities of TiAl3-type intermetallics in AlPtTi system. *Computational Materials Science*, **2013**, 68, 229-233	3.2	31
76	Phase stability and anisotropic elastic properties of the HfAl intermetallics: A DFT calculation. *Computational Materials Science*, **2015**, 110, 10-19	3.2	30
75	Surface evolution and growth kinetics of Ti6Al4V alloy in pack boriding. *Journal of Alloys and Compounds*, **2018**, 742, 690-701	5.7	28
74	Anisotropic elasticity and thermal conductivities of (β)-LiAlSi2O6 from the first-principles calculation. *Journal of Alloys and Compounds*, **2018**, 756, 40-49	5.7	27
73	Anisotropies in elastic properties and thermal conductivities of trigonal TM2C (TM = V, Nb, Ta) carbides. *Solid State Sciences*, **2019**, 98, 106027	3.4	26

72	Structural, electronic, and elastic properties of orthorhombic, hexagonal, and cubic Cu3Sn intermetallic compounds in Sn□Cu lead-free solder. *Journal of Physics and Chemistry of Solids*, **2020**, 138, 109253	3.9	25
71	Predictions of phase stabilities, electronic structures and optical properties of potential superhard WB3. *Ceramics International*, **2019**, 45, 3341-3349	5.1	25
70	Surface characterization and diffusion model of pack borided TB2 titanium alloy. *Ceramics International*, **2018**, 44, 18429-18437	5.1	22
69	Anisotropic elastic properties of MB (M = Cr, Mo, W) monoborides: a first-principles investigation. *Philosophical Magazine*, **2016**, 96, 972-990	1.6	22
68	Phase stability, elastic anisotropy and electronic structure of cubic MAl2(M = Mg, Ca, Sr and Ba) Laves phases from first-principles calculations. *Materials Research Express*, **2016**, 3, 106505	1.7	21
67	Elastic anisotropies and thermal properties of cubic TMIr (TM=Sc, Y, Lu, Ti, Zr and Hf): A DFT calculation. *Materials Research Express*, **2019**, 6, 086574	1.7	18
66	Structural and anisotropic elastic properties of hexagonal MP (M = Ti, Zr, Hf) monophosphides determined by first-principles calculations. *Philosophical Magazine*, **2016**, 96, 3654-3670	1.6	18
65	Structural properties, phase stability, elastic properties and electronic structures of Cu□Ti intermetallics. *Philosophical Magazine*, **2015**, 95, 3535-3553	1.6	17
64	Characteristics, wear and corrosion properties of borided pure titanium by pack boriding near □s□ phase transition temperature. *Ceramics International*, **2020**, 46, 16380-16387	5.1	17
63	The mechanical and thermodynamic properties of ZrTM (TM=Fe, Ru and Os) intermetallics under pressure and temperature: A first-principles predictions. *Journal of Physics and Chemistry of Solids*, **2020**, 142, 109465	3.9	17
62	Microstructure, Growth Kinetics and Some Mechanical Properties of Boride Layers Produced on Pure Titanium by Molten-Salt Boriding. *Journal of Materials Engineering and Performance*, **2017**, 26, 4544-4555	1.6	16
61	Structural and anisotropic elastic properties of Zintl M2Pb (M=Ca, Sr and Ba) compounds as a function of pressure. *Journal of Alloys and Compounds*, **2014**, 614, 334-344	5.7	16
60	Phase stability, anisotropic elastic properties and electronic structures of C15-type Laves phases ZrM2 (M = Cr, Mo and W) from first-principles calculations. *Philosophical Magazine*, **2017**, 97, 2406-2424	1.6	15
59	Characteristics of surface layers on Ti6Al4V alloy borided with CeO2 near the transition temperature. *Journal of Alloys and Compounds*, **2018**, 769, 1-9	5.7	15
58	Predictions of structural, electronic, mechanical, and thermodynamic properties of TMBCs (TM□□Ti, Zr, and Hf) ceramics. *Journal of the American Ceramic Society*, **2020**, 103, 5232-5247	3.8	14
57	First-principles predictions of electronic, elastic, and optical properties of ScBC and YBC ternary cermet phases. *Vacuum*, **2020**, 179, 109488	3.7	14
56	A first-principles investigation of structural properties, electronic structures and optical properties of □and □LiAl(SiO3)2. *Ceramics International*, **2017**, 43, 13948-13955	5.1	14
55	Stability and electronic structures of the Ti Zn intermetallic compounds: A DFT calculation. *Physica B: Condensed Matter*, **2019**, 560, 41-45	2.8	13

54	Anisotropy of elastic and thermal properties of TMOs2 (TM = Sc, Y, Ti, Zr and Hf) from first-principles explorations. *Materials Research Express*, **2019**, 6, 116569	1.7	13
53	Stability, elastic properties and electronic structures of L12-ZrAl3 and D022-ZrAl3 up to 40GPa. *Journal of Physics and Chemistry of Solids*, **2014**, 75, 535-542	3.9	13
52	First-principles calculations of optical properties of Mg2Pb. *Science China: Physics, Mechanics and Astronomy*, **2014**, 57, 233-238	3.6	13
51	Characterization and growth kinetics of boride layers on Ti-5Mo-5V-8Cr-3Al alloy by pack boriding with CeO2. *Materials Characterization*, **2020**, 164, 110362	3.9	12
50	Constitutive Equations, Processing Maps, and Microstructures of Pb-Mg-Al-B-0.4Y Alloy under Hot Compression. *Journal of Materials Engineering and Performance*, **2020**, 29, 607-619	1.6	12
49	Dynamic Recrystallization and Processing Map of Pb-30Mg-9Al-1B Alloy During Hot Compression. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2017**, 48, 3419-3431	2.3	9
48	Theoretical predictions of thermodynamic and electronic properties of TiM (M = Fe, Ru and Os). *Physica B: Condensed Matter*, **2019**, 573, 13-21	2.8	9
47	Insight into structural, electronic, elastic and thermal properties of A15-type Nb3X (X = Si, Ge, Sn and Pb) compounds. *Materials Today Communications*, **2020**, 25, 101410	2.5	9
46	Hot Deformation and Processing Map of Pb-Mg-10Al-1B Alloy. *Journal of Materials Engineering and Performance*, **2013**, 22, 3049-3054	1.6	9
45	Structural, electronic, mechanical, and thermodynamic properties of ultra-high-temperature ceramics □and □YAlB4: A first-principles study. *Ceramics International*, **2021**, 47, 10079-10088	5.1	9
44	Explorations of elastic anisotropies and thermal properties of the hexagonal TMSi2 (TM = Cr, Mo, W) silicides from first-principles calculations. *Materials Today Communications*, **2021**, 27, 102474	2.5	9
43	First-principles investigations on Pb□a intermetallic compounds. *Computational Materials Science*, **2014**, 92, 258-266	3.2	8
42	Insights into structural stability, electronic structure, and elastic and thermodynamic properties of A15-type Mo3X (X = Si, Ge, and Sn) compounds based on first-principles predictions. *Journal of Physics and Chemistry of Solids*, **2021**, 151, 109925	3.9	8
41	Flow Behavior, Dynamic Recrystallization and Processing Map of Mg-20Pb-1.6Al-0.4B Alloy. *Journal of Materials Engineering and Performance*, **2017**, 26, 2439-2451	1.6	7
40	The interstitial diffusion behaviors and mechanisms of boron in □Ti and □Ti: A first-principles calculation. *Computational Materials Science*, **2020**, 184, 109866	3.2	7
39	First-principles predictions of anisotropies in elasticity and sound velocities of CsCl-type refractory intermetallics: TiTM, ZrTM and HfTM (TM = Fe, Ru, Os). *Philosophical Magazine*, **2019**, 99, 2681-2702	1.6	7
38	Calculated structure, elastic and electronic properties of Mg2Pb at high pressure. *Journal Wuhan University of Technology, Materials Science Edition*, **2012**, 27, 377-381	1	7
37	Insight into anisotropies in mechanical and thermal properties of AGdS2 (A = alkali metals) ternary gadolinium sulfides. *Materials Today Communications*, **2021**, 26, 101991	2.5	7

36	Insights into electronic and optical properties of AGdS2 (A = Li, Na, K, Rb and Cs) ternary gadolinium sulfides. *Optical Materials*, **2021**, 114, 110963	3.3	7
35	Explorations of electronic, elastic and thermal properties of tetragonal TM4N3 (TM=V, Nb and Ta) nitrides. *Materials Today Communications*, **2021**, 26, 101723	2.5	7
34	First-principles calculations of electronic, optical, phononic and thermodynamic properties of C40-type TMSi2 (TM = Cr, Mo, W) disilicides. *Vacuum*, **2021**, 191, 110324	3.7	7
33	Insight of structural stability, elastic anisotropies and thermal conductivities of Y, Sc doped Mg2Pb from first-principles calculations. *Chemical Physics Letters*, **2020**, 756, 137833	2.5	6
32	Revealing the elastic properties and anisotropies of Mg2X(X = Si, Ge and Sn) with different structures from a first-principles calculation. *Materials Today Communications*, **2020**, 24, 101337	2.5	5
31	Adsorption of fluorine and chlorine on Mg (0001) surface: A density functional theory investigation. *Transactions of Nonferrous Metals Society of China*, **2014**, 24, 1844-1852	3.3	5
30	Elastic properties, fracture toughness, ideal tensile strength and thermal conductivities of the stable hexagonal WB2, W2B5, WB3 and WB4. *Applied Physics A: Materials Science and Processing*, **2022**, 128, 1	2.6	5
29	Theoretical insights into anisotropies in elastic and thermal properties of ternary □M4AlN3 (M = V, Nb, Ta) nitrides by first-principles calculations. *Chemical Physics Letters*, **2021**, 783, 139088	2.5	5
28	Corrosion behavior of Pb-39Mg-10Al-1.5B alloy in sodium halide solutions. *Journal of Alloys and Compounds*, **2017**, 729, 1108-1117	5.7	4
27	The electronic structure and phase diagram of chlorine adsorption on Mg (0 0 0 1) surface. *Computational Materials Science*, **2014**, 84, 108-114	3.2	4
26	Elastic anisotropies, thermal conductivities and tensile properties of MAX phases Zr2AlC and Zr2AlN: A first-principles calculation. *Vacuum*, **2021**, 110715	3.7	4
25	The anisotropic properties and Debye temperatures of Ti-Zn compounds: a first-principles calculation. *Materials Research Express*, **2019**, 6, 116528	1.7	3
24	Thermodynamics properties and thermal conductivity of Mg2Pb at high pressure. *Science China: Physics, Mechanics and Astronomy*, **2013**, 56, 1854-1860	3.6	3
23	Electronic, elastic, and thermal properties, fracture toughness, and damage tolerance of TM5Si3B (TM□□V and Nb) MAB phases. *International Journal of Refractory Metals and Hard Materials*, **2022**, 103, 105781	4.1	3
22	Experimental investigations of TB2 alloy by pack boriding with rare-earth oxides. *Philosophical Magazine Letters*, **2018**, 98, 521-526	1	3
21	First-principles exploration of elastic anisotropy and thermal properties of the C40-type VSi2, NbSi2, and TaSi2 disilicides. *Materials Today Communications*, **2021**, 29, 102818	2.5	3
20	First-principles study on the elasticity and thermal properties of heavy Fermi compounds CePtSix (X=1,2,3). *Physica B: Condensed Matter*, **2022**, 624, 413371	2.8	3
19	First-principles calculations of structure and electronic properties of aluminum doped by Ge, Sn and Pb. *Physica B: Condensed Matter*, **2018**, 547, 6-11	2.8	2

18	Effects of temperature and pressure on the mechanical and thermodynamic properties of high-boride WB4 from first-principles predictions. *Materials Today Communications*, **2022**, 30, 103187	2.5	2
17	Theoretical insights to elastic and thermal properties of WB4 tetraborides: A first-principles calculation. *Vacuum*, **2021**, 110731	3.7	2
16	Theoretical explorations of structure, mechanical properties, fracture toughness, electronic properties, and thermal conductivity of Ag-doped η-Cu6Sn5. *Intermetallics*, **2022**, 141, 107437	3.5	2
15	First-principles investigation on the structures, energies and electronic properties of low-index surfaces of Mg2Pb. *Materials Chemistry and Physics*, **2021**, 260, 124028	4.4	2
14	Hardness gradient layer on pure titanium based on the prefabricated TiB whiskers. *Ceramics International*, **2021**, 47, 25142-25146	5.1	2
13	Hot compressive deformation behaviour and constitutive equations of MgPbAlBO.4Sc alloy. *Philosophical Magazine*,1-22	1.6	2
12	Structural stability, electronic and optical properties of MAX-phase ternary nitrides TM4AlN3 (TM = V, Nb, and Ta) using the first-principles explorations. *Vacuum*, **2021**, 193, 110529	3.7	2
11	Theoretical insights on elastic anisotropy and thermal anisotropy of TM5Al3C (TM= Zr, Hf, and Ta) carbides. *Vacuum*, **2022**, 200, 110989	3.7	2
10	Elastic properties and thermal conductivities of fluor-, chlor- and brom-barium apatites predicted by first-principles simulations. *Philosophical Magazine*, **2017**, 97, 1708-1728	1.6	1
9	Effect of Yttrium on the Microstructure and Properties of Pt-Ir Electrical Contact Materials. *IOP Conference Series: Materials Science and Engineering*, **2017**, 250, 012017	0.4	1
8	Theoretical predictions of the electronic, optical and thermodynamic properties of the C40-type TMSi2 (TM=V, Nb and Ta) disilicides. *Materials Today Communications*, **2022**, 30, 103115	2.5	1
7	Revealing effects of common nonmetallic impurities on the stability and strength of Cu/Sn solder joints: A first-principles investigation. *Vacuum*, **2022**, 200, 110997	3.7	1
6	Adhesion, stability and electronic properties of TiB (100)/α-Ti (0001) coherent interface: Insights from a first-principles investigation. *Surfaces and Interfaces*, **2022**, 30, 101974	4.1	1
5	Microstructure and mechanical properties of Pb-40 Mg-10Al-1B-Y alloys. *Materials Today Communications*, **2021**, 27, 102371	2.5	0
4	Effects of Yttrium on the Microstructure and Corrosion Behavior of Pb-39Mg-10Al-1B-Y Alloys. *Journal of Materials Engineering and Performance*, **2021**, 30, 77-88	1.6	0
3	Insights of electronic structures, mechanical properties and thermal conductivities of TM5SiB2 (TM=V, Nb, and Ta) MAB phases. *Philosophical Magazine*,1-22	1.6	0
2	First-Principles Investigation of Elasticity, Thermal and Electronic Properties of Intermetallics Formed at the Interface of Al-Cu Composites. *Journal of Electronic Materials*,1	1.9	
1	Effects of vacancies on structural, electronic, mechanical, and thermodynamic properties of C40-VSi2. *Philosophical Magazine*,1-17	1.6	