Yonghua Duan

List of Publications by Year
in descending order

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Version: 2024-02-01

97 papers	2,522 citations	201385 27 h-index	243296 44 g-index
97 all docs	97 docs citations	97 times ranked	1022 citing authors

#	Article	IF	Citations
1	Anisotropic elastic properties of the Caâ€“Pb compounds. Journal of Alloys and Compounds, 2014, 595, 14-21.	2.8	140
2	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.	2.8	105
3	Stability, elastic properties and electronic structures of the stable Zrâ€“Al intermetallic compounds: A first-principles investigation. Journal of Alloys and Compounds, 2014, 590, 50-60.	2.8	97
4	Structural, anisotropic elastic and thermal properties of MB (M=Ti, Zr and Hf) monoborides. Ceramics International, 2015, 41, 6831-6843.	2.3	92
5	Electronic structures, mechanical and thermodynamic properties of cubic alkaline-earth hexaborides from first principles calculations. Journal of Alloys and Compounds, 2015, 635, 213-224.	2.8	87
6	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.	2.8	84
7	A first-principles prediction of anisotropic elasticity and thermal properties of potential superhard WB3. Ceramics International, 2018, 44, 14053-14062.	2.3	84
8	Developed constitutive models, processing maps and microstructural evolution of Pb-Mg-10Al-0.5B alloy. Materials Characterization, 2017, 129, 353-366.	1.9	59
9	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.	2.8	56
10	Structural properties, elastic anisotropies and thermal conductivities of tetragonal LnB2C2 (Ln =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	2.3	56
11	Structural, electronic, and elastic properties of orthorhombic, hexagonal, and cubic Cu3Sn intermetallic compounds in Snâ€“Cu lead-free solder. Journal of Physics and Chemistry of Solids, 2020, 138, 109253.	1.9	54
12	Structural properties, electronic structures and optical properties of WB2 with different structures: A theoretical investigation. Ceramics International, 2018, 44, 11438-11447.	2.3	52
13	Anisotropies in elastic properties and thermal conductivities of trigonal TM2C (TM = V, Nb, Ta) carbides. Solid State Sciences, 2019, 98, 106027.	1.5	49
14	Characteristics, wear and corrosion properties of borided pure titanium by pack boriding near Î± â†' Î² phase transition temperature. Ceramics International, 2020, 46, 16380-16387.	2.3	48
15	Thermodynamic properties and thermal conductivities of TiAl3-type intermetallics in Alâ€“Ptâ€“Ti system. Computational Materials Science, 2013, 68, 229-233.	1.4	46
16	Ab-initio investigations on elastic properties in L12 structure Al3Sc and Al3Y under high pressure. Journal of Alloys and Compounds, 2014, 585, 587-593.	2.8	44
17	Surface evolution and growth kinetics of Ti6Al4V alloy in pack boriding. Journal of Alloys and Compounds, 2018, 742, 690-701.	2.8	42
18	Electronic, elastic, and thermal properties, fracture toughness, and damage tolerance of TM5Si3B (TMÂ=ÂV and Nb) MAB phases. International Journal of Refractory Metals and Hard Materials, 2022, 103, 105781.	1.7	42

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19	Phase stability and anisotropic elastic properties of the Hfâ€“Al intermetallics: A DFT calculation. Computational Materials Science, 2015, 110, 10-19.	1.4	41
20	Surface characterization and diffusion model of pack borided TB2 titanium alloy. Ceramics International, 2018, 44, 18429-18437.	2.3	41
21	Anisotropic elasticity and thermal conductivities of (Î±, Î², Î³)-LiAlSi2O6 from the first-principles calculation. Journal of Alloys and Compounds, 2018, 756, 40-49.	2.8	39
22	Elastic anisotropies, thermal conductivities and tensile properties of MAX phases Zr2AlC and Zr2AlN: A first-principles calculation. Vacuum, 2022, 196, 110715.	1.6	39
23	Predictions of phase stabilities, electronic structures and optical properties of potential superhard WB3. Ceramics International, 2019, 45, 3341-3349.	2.3	35
24	Predictions of structural, electronic, mechanical, and thermodynamic properties of TMBCs (TMÂ=ÂTi, Zr,) Tj ETQq0 0 0 rgBT /Overlock 10	1.9	33
25	Anisotropic elastic properties of MB (M = Cr, Mo, W) monoborides: a first-principles investigation. Philosophical Magazine, 2016, 96, 972-990.	0.7	31
26	Structural properties, phase stability, elastic properties and electronic structures of Cuâ€“Ti intermetallics. Philosophical Magazine, 2015, 95, 3535-3553.	0.7	29
27	First-principles predictions of electronic, elastic, and optical properties of ScBC and YBC ternary cermet phases. Vacuum, 2020, 179, 109488.	1.6	29
28	Characterization and growth kinetics of boride layers on Ti-5Mo-5V-8Cr-3Al alloy by pack boriding with CeO2. Materials Characterization, 2020, 164, 110362.	1.9	29
29	Anisotropic Elastic and Thermal Properties of M2InX (M = Ti, Zr and X = C, N) Phases: A First-Principles Calculation. Metals, 2022, 12, 1111.	1.0	28
30	Theoretical insights on elastic anisotropy and thermal anisotropy of TM5Al3C (TM= Zr, Hf, and Ta) carbides. Vacuum, 2022, 200, 110989.	1.6	27
31	Insights into electronic and optical properties of AGdS2 (A = Li, Na, K, Rb and Cs) ternary gadolinium sulfides. Optical Materials, 2021, 114, 110963.	1.7	26
32	Phase stability, anisotropic elastic properties and electronic structures of C15-type Laves phases ZrM₂(MÂ=ÂCr, Mo and W) from first-principles calculations. Philosophical Magazine, 2017, 97, 2406-2424.	0.7	25
33	Structural and anisotropic elastic properties of hexagonal MP (M = Ti, Zr, Hf) monophosphides determined by first-principles calculations. Philosophical Magazine, 2016, 96, 3654-3670.	0.7	24
34	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.	1.2	24
35	Theoretical insights into anisotropies in elastic and thermal properties of ternary Î²-M4AlN3 (MÂ=ÂV, Nb,) Tj ETQq1 1 0.784314 rgBT	1.2	24
36	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.	1.9	24

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37	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.	2.8	23
38	Phase stability, elastic anisotropy and electronic structure of cubic MAl₂(M = Mg, Ca, Sr) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.8	23
39	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.	0.8	23
40	Stability and electronic structures of the Ti Zn intermetallic compounds: A DFT calculation. Physica B: Condensed Matter, 2019, 560, 41-45.	1.3	23
41	A first-principles investigation of structural properties, electronic structures and optical properties of Î²- and Î³-LiAl(SiO3)2. Ceramics International, 2017, 43, 13948-13955.	2.3	22
42	Characteristics of surface layers on Ti6Al4V alloy borided with CeO2 near the transition temperature. Journal of Alloys and Compounds, 2018, 769, 1-9.	2.8	22
43	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.	1.2	22
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.	0.9	21
45	First-principles calculations of electronic, optical, phononic and thermodynamic properties of C40-type TMSi2 (TM = Cr, Mo, W) disilicides. Vacuum, 2021, 191, 110324.	1.6	21
46	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.	1.1	20
47	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.	1.9	19
48	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.	1.1	19
49	The interstitial diffusion behaviors and mechanisms of boron in Î±-Ti and Î²-Ti: A first-principles calculation. Computational Materials Science, 2020, 184, 109866.	1.4	19
50	Insights of electronic structures, mechanical properties and thermal conductivities of TM₅SiB₂(TM=V, Nb, and Ta) MAB phases. Philosophical Magazine, 2022, 102, 1628-1649.	0.7	18
51	First-principles calculations of optical properties of Mg2Pb. Science China: Physics, Mechanics and Astronomy, 2014, 57, 233-238.	2.0	16
52	First-principles investigations on Pbâ€“Ba intermetallic compounds. Computational Materials Science, 2014, 92, 258-266.	1.4	16
53	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.	0.8	16
54	Structural, electronic, mechanical, and thermodynamic properties of ultra-high-temperature ceramics Î±- and Î²-YAlB4: A first-principles study. Ceramics International, 2021, 47, 10079-10088.	2.3	16

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55	Theoretical explorations of structure, mechanical properties, fracture toughness, electronic properties, and thermal conductivity of Ag-doped Î·â€²-Cu6Sn5. Intermetallics, 2022, 141, 107437.	1.8	16
56	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.	1.2	15
57	Theoretical predictions of thermodynamic and electronic properties of TiM (Mâ€¯=â€¯Fe, Ru and Os). Physica B: Condensed Matter, 2019, 573, 13-21.	1.3	15
58	Insight of structural stability, elastic anisotropies and thermal conductivities of Y, Sc doped Mg2Pb from first-principles calculations. Chemical Physics Letters, 2020, 756, 137833.	1.2	15
59	Insight into structural, electronic, elastic and thermal properties of A15-type Nb3X (X = Si, Ge, Sn and) Tj ETQq1 1 0.784314 rgBT /Ov	0.9	15
60	Revealing effects of common nonmetallic impurities on the stability and strength of Cuâ€“Sn solder joints: A first-principles investigation. Vacuum, 2022, 200, 110997.	1.6	15
61	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.	1.9	14
62	Hot compressive deformation behaviour and constitutive equations of Mgâ€“Pbâ€“Alâ€“1Bâ€“0.4Sc alloy. Philosophical Magazine, 2021, 101, 2355-2376.	0.7	14
63	Structural stability, electronic and optical properties of MAX-phase ternary nitrides Î²-TM4AlN3 (TM = V,) Tj ETQq1 1 0.784314 rgBT /O	1.6	14
64	First-principles predictions of anisotropies in elasticity and sound velocities of CsCl-type refractory intermetallics: TiTM, ZrTM and HfTM (TMâ€‰=â€‰Fe, Ru, Os). Philosophical Magazine, 2019, 99, 2681-2702.	0.7	13
65	Insight into anisotropies in mechanical and thermal properties of AGdS2 (Aâ€‰=â€‰alkali metals) ternary gadolinium sulfides. Materials Today Communications, 2021, 26, 101991.	0.9	13
66	First-principles exploration of elastic anisotropy and thermal properties of the C40-type VSi2, NbSi2, and TaSi2 disilicides. Materials Today Communications, 2021, 29, 102818.	0.9	13
67	Hot Deformation and Processing Map of Pb-Mg-10Al-1B Alloy. Journal of Materials Engineering and Performance, 2013, 22, 3049-3054.	1.2	12
68	Microstructure and high-temperature oxidation behaviors of surface layer on TA2 pure titanium by boriding and aluminizing two-steps method. Ceramics International, 2022, 48, 5646-5654.	2.3	12
69	Wear and corrosion properties of a Bâ€“Al composite layer on pure titanium. Ceramics International, 2022, 48, 12038-12047.	2.3	12
70	The electronic structure and phase diagram of chlorine adsorption on Mg (0001) surface. Computational Materials Science, 2014, 84, 108-114.	1.4	11
71	Corrosion behavior of Pb-39Mg-10Al-1.5B alloy in sodium halide solutions. Journal of Alloys and Compounds, 2017, 729, 1108-1117.	2.8	11
72	Revealing the elastic properties and anisotropies of Mg2X(Xâ€‰=â€‰Si, Ge and Sn) with different structures from a first-principles calculation. Materials Today Communications, 2020, 24, 101337.	0.9	11

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73	Hardness gradient layer on pure titanium based on the prefabricated TiB whiskers. Ceramics International, 2021, 47, 25142-25146.	2.3	11
74	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.	1.7	10
75	Calculated structure, elastic and electronic properties of Mg2Pb at high pressure. Journal Wuhan University of Technology, Materials Science Edition, 2012, 27, 377-381.	0.4	9
76	The anisotropic properties and Debye temperatures of Ti-Zn compounds: a first-principles calculation. Materials Research Express, 2019, 6, 116528.	0.8	9
77	First-principles investigation on the structures, energies and electronic properties of low-index surfaces of Mg2Pb. Materials Chemistry and Physics, 2021, 260, 124028.	2.0	9
78	Theoretical insights to elastic and thermal properties of WB4 tetraborides: A first-principles calculation. Vacuum, 2022, 196, 110731.	1.6	9
79	Explorations of electronic, elastic and thermal properties of tetragonal TM4N3 (TM=V, Nb and Ta) nitrides. Materials Today Communications, 2021, 26, 101723.	0.9	8
80	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.	1.2	8
81	Microstructure and some properties of powder-pack borided Tiâ€“5Moâ€“5Vâ€“8Crâ€“3Al alloy with special attention to the microstructure at the interface TiB/substrate. Ceramics International, 2022, 48, 24346-24354.	2.3	8
82	Experimental investigations of TB2 alloy by pack boriding with rare-earth oxides. Philosophical Magazine Letters, 2018, 98, 521-526.	0.5	7
83	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.	1.3	7
84	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.	0.9	6
85	Revealing the interface characteristic of the semi-coherent Co(111)/WC(0001) interface: a first principles investigation. Philosophical Magazine, 2022, 102, 2031-2055.	0.7	5
86	Thermodynamics properties and thermal conductivity of Mg2Pb at high pressure. Science China: Physics, Mechanics and Astronomy, 2013, 56, 1854-1860.	2.0	4
87	Adhesion strength, stability and electronic properties of Î±-Mg/Mg2Pb interface from first-principles calculation. Journal of Materials Research, 2022, 37, 1859-1867.	1.2	4
88	Revealing boron adsorption on the Î±-Ti(0001) surface by first-principles calculations. Philosophical Magazine, 2022, 102, 1873-1890.	0.7	4
89	First-principles calculations of structure and electronic properties of aluminum doped by Ge, Sn and Pb. Physica B: Condensed Matter, 2018, 547, 6-11.	1.3	3
90	Adhesion, stability and electronic properties of TiB (100)/ Î±-Ti (0001) coherent interface: Insights from a first-principles investigation. Surfaces and Interfaces, 2022, 30, 101974.	1.5	3

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91	Effects of vacancies on structural, electronic, mechanical, and thermodynamic properties of C40-VSi ₂. Philosophical Magazine, 2022, 102, 1505-1521.	0.7	3
92	Effect of Yttrium on the Microstructure and Properties of Pt-Ir Electrical Contact Materials. IOP Conference Series: Materials Science and Engineering, 2017, 250, 012017.	0.3	2
93	Theoretical predictions of the electronic, optical and thermodynamic properties of the C40-type TMSi2 (TMÂ=ÂV, Nb and Ta) disilicides. Materials Today Communications, 2022, 30, 103115.	0.9	2
94	First-Principles Investigation of Elasticity, Thermal and Electronic Properties of Intermetallics Formed at the Interface of Al-Cu Composites. Journal of Electronic Materials, 2022, 51, 3782-3797.	1.0	2
95	Structural stability, electronic and optical properties of Zr-Al-N ternary nitrides using the first-principles explorations. Materials Today Communications, 2022, 32, 103962.	0.9	2
96	Elastic properties and thermal conductivities of fluor-, chlor- and brom-barium apatites predicted by first-principles simulations. Philosophical Magazine, 2017, 97, 1708-1728.	0.7	1
97	Microstructure and mechanical properties of Pb-40 Mg-10Al-1B-Y alloys. Materials Today Communications, 2021, 27, 102371.	0.9	1