Xiao-Yu Chong

List of Publications by Year
in descending order

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70	2,152	236925	243625
papers	citations	25	44
		h-index	g-index

71	71	71	1805
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Enhanced thermoelectric performance in inorganic CsSnI3 perovskite by doping with PbI2. Materials Letters, 2022, 308, 131127.	2.6	8
2	Lattice stability, mechanical and thermal properties of a new class of multicomponent (Fe, Mo, W)6C Î· carbides with different atomic site configurations. Ceramics International, 2022, 48, 5107-5118.	4.8	8
3	Morphology, thermal stability, electronic structure and mechanical properties of Î±-AlFeMnSi phases with varying Mn/Fe atomic ratios: Experimental studies and DFT calculations. Journal of Alloys and Compounds, 2022, 901, 163523.	5.5	17
4	Exploring the solution strengthening effect of 33 alloying elements in Pt-based alloys by high-throughput first-principles calculations. Journal of Applied Physics, 2022, 131, .	2.5	4
5	Changes of alloying elements on elasticity and solid solution strengthening of Î±-Ti alloys: a comprehensive high-throughput first-principles calculations. Rare Metals, 2022, 41, 2719-2731.	7.1	13
6	Design of Fe2B-based ductile high temperature ceramics: First-principles calculations and experimental validation. Ceramics International, 2022, 48, 27163-27173.	4.8	11
7	Investigation on elastic properties and electronic structure of dilute Ir-based alloys by first-principles calculations. Journal of Alloys and Compounds, 2021, 850, 156548.	5.5	18
8	Balance between strength and ductility of dilute Fe2B by high-throughput first-principles calculations. Ceramics International, 2021, 47, 4758-4768.	4.8	16
9	Stability, electronic structure, mechanical properties and lattice thermal conductivity of FeS and FeS₂ polymorphs. Modern Physics Letters B, 2021, 35, 2150225.	1.9	1
10	Numerical Optimization for the Geometric Configuration of Ceramics Perform in HCCI/ZTAP Wear-Resistant Composites Based on Actual Particle Model. Nanoscale Research Letters, 2021, 16, 71.	5.7	0
11	Correlation analysis of materials properties by machine learning: illustrated with stacking fault energy from first-principles calculations in dilute fcc-based alloys. Journal of Physics Condensed Matter, 2021, 33, 295702.	1.8	13
12	Highâ€entropy ferroelastic rareâ€earth tantalite ceramic: (Y_{0.2}Ce_{0.2}Sm_{0.2}Gd_{0.2}Dy_{0.2})TaO₄ Journal of the American Ceramic Society, 2021, 104, 5873-5882.	3.8	49
13	Probing the mechanical properties of ordered and disordered Pt-Ir alloys by first-principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 405, 127424.	2.1	17
14	Firstâ€principles study of thermophysical properties of polymorphous YTaO₄ ceramics. Journal of the American Ceramic Society, 2021, 104, 6467-6480.	3.8	20
15	Exploring crystal structures, stability and mechanical properties of Fe, Mn-containing intermetallics in Al-Si Alloy by experiments and first-principles calculations. Journal of Alloys and Compounds, 2021, 876, 160022.	5.5	28
16	Thermodynamic properties of the Yb-Sb system predicted from first-principles calculations. Acta Materialia, 2021, 217, 117169.	7.9	34
17	First-Principles Calculations of Thermal and Electrical Transport Properties of bcc and fcc Dilute Feâ€“X (X = Al, Co, Cr, Mn, Mo, Nb, Ni, Ti, V, and W) Binary Alloys. Metals, 2021, 11, 1988.	2.3	6
18	Thermal properties of Y1â^'xMgxTaO4â^'x/2 ceramics via anion sublattice adjustment. Rare Metals, 2020, 39, 545-554.	7.1	22

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19	Sub-1.4eV bandgap inorganic perovskite solar cells with long-term stability. Nature Communications, 2020, 11, 151.	12.8	92
20	The thermoâ€mechanical properties and ferroelastic phase transition of RENbO₄ (REÂ=ÂY, La,) Tj ETQq0 0 0 rgBT /Overlock	3.8	36
21	Effects of the alloying element on the stacking fault energies of dilute Ir-based superalloys: A comprehensive first-principles study. Journal of Materials Research, 2020, 35, 2718-2725.	2.6	7
22	Anisotropic mechanical properties and electronic structures of transition metal carbonitrides M2CN (Mâ€‰=â€‰V, Ti, Ta, Nb, Hf and Zr) by first-principles calculations. Applied Physics A: Materials Science and Processing, 2020, 126, 1.	2.3	4
23	Effect of solution treatment on mechanical properties and microstructure of welded joints of Fe-29Mn-9Al-0.9C low-density steel. Journal of Micromechanics and Molecular Physics, 2020, 05, 2050006.	1.2	6
24	Investigation of the thermophysical properties of (Y1-xYbx)TaO4 ceramics. Journal of the European Ceramic Society, 2020, 40, 3111-3121.	5.7	18
25	Mechanical and thermal properties of RETaO4 (RE = Yb, Lu, Sc) ceramics with monoclinic-prime phase. Journal of Materials Science and Technology, 2020, 52, 20-28.	10.7	40
26	Investigation on the stability, electronic, optical, and mechanical properties of novel calcium carbonate hydrates via firstâ€principles calculations. International Journal of Quantum Chemistry, 2020, 120, e26219.	2.0	8
27	Rapid screening of alloy elements to improve the elastic properties of dilute Pt-based alloys: High-throughput first-principles calculations and modeling. Journal of Applied Physics, 2020, 128, .	2.5	16
28	The effect of ZrO₂ alloying on the microstructures and thermal properties of DyTaO₄ for highâ€temperature application. Journal of the American Ceramic Society, 2019, 102, 889-895.	3.8	16
29	The Effects of Laser Remelting on the Microstructure and Performance of Bainitic Steel. Metals, 2019, 9, 912.	2.3	10
30	An alternative approach to predict Seebeck coefficients: Application to La3â^'xTe4. Scripta Materialia, 2019, 169, 87-91.	5.2	9
31	Electronic, mechanical and hydrogen storage properties of novel Mg3N2. Journal of Alloys and Compounds, 2019, 800, 8-15.	5.5	7
32	Theoretical and experimental investigations of mechanical properties for polymorphous YTaO₄ceramics. Journal of the American Ceramic Society, 2019, 102, 7656-7664.	3.8	30
33	Multipoint Defect Synergy Realizing the Excellent Thermoelectric Performance of nâ€Type Polycrystalline SnSe via Re Doping. Advanced Functional Materials, 2019, 29, 1902893.	14.9	73
34	Tailoring the anisotropic mechanical properties of hexagonal M7X3 (M=Fe, Cr, W, Mo; X=C, B) by multialloying. Acta Materialia, 2019, 169, 193-208.	7.9	74
35	First-principles study of pressure-induced phase transformations in thermoelectric Mg2Si. Journal of Alloys and Compounds, 2019, 773, 988-996.	5.5	9
36	Stability, mechanical and electronic properties of ceramic interphases in biomedical composites via first-principles calculations. Ceramics International, 2018, 44, 9656-9663.	4.8	8

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37	Exploring the intrinsic ductile metastable Fe-C compounds: Complex chemical bonds, anisotropic elasticity and variable thermal expansion. Journal of Alloys and Compounds, 2018, 745, 196-211.	5.5	32
38	Effect of Al³⁺ doping on mechanical and thermal properties of DyTaO₄ as promising thermal barrier coating application. Journal of the American Ceramic Society, 2018, 101, 1818-1823.	3.8	32
39	Synthesis and thermophysical properties of RETa₃O₉ (REÂ=ÂCe, Nd, Sm, Eu, Gd,) Tj ETQq1 1 0.784314 rgB 1266-1278.	3.8	93
40	Enhanced thermoelectric properties of bismuth telluride bulk achieved by telluride-spilling during the spark plasma sintering process. Scripta Materialia, 2018, 143, 90-93.	5.2	77
41	Interface transition layer interaction mechanism for ZTA_P/HCCI composites. Science and Engineering of Composite Materials, 2018, 25, 881-890.	1.4	12
42	Quasiharmonic calculations of thermodynamic properties for La3â^'xTe4 system. Computational Materials Science, 2018, 142, 417-426.	3.0	6
43	A first-principles calculation of structural, mechanical, thermodynamic and electronic properties of binary Niâ€“Y compounds. RSC Advances, 2018, 8, 41575-41586.	3.6	17
44	Investigation on microstructures and thermo-physical properties of ferroelastic (Y1-xDyx)TaO4 ceramics. Materialia, 2018, 4, 478-486.	2.7	25
45	Revealing the stability, elastic properties and electronic structures of Pd-V intermetallics via first principle calculations. AIP Advances, 2018, 8, .	1.3	6
46	Understanding the Intrinsic P-Type Behavior and Phase Stability of Thermoelectric Î±-Mg₃Sb₂. ACS Applied Energy Materials, 2018, 1, 6600-6608.	5.1	28
47	Wear Resistance Mechanism of ZTAP/HCCI Composites with a Honeycomb Structure. Metals, 2018, 8, 588.	2.3	19
48	Excellent ZT achieved in Cu_{1.8}S thermoelectric alloys through introducing rare-earth trichlorides. Journal of Materials Chemistry A, 2018, 6, 14440-14448.	10.3	39
49	Properties of Feâ€“Mnâ€“Al alloys with different Mn contents using density functional theory. Rare Metals, 2018, , 1.	7.1	1
50	The rattler effect of phonon propagation in defect-fluorite Dy3(Nb1-xTix)O7-x/2. Ceramics International, 2018, 44, 21998-22002.	4.8	9
51	Exploring accurate structure, composition and thermophysical properties of Î· carbides in 17.90â€¯wt% W-4.15â€¯wt% Cr-1.10â€¯wt% V-0.69â€¯wt% C steel. Scripta Materialia, 2018, 154, 149-153.	5.2	18
52	Highly Enhanced Thermoelectric Properties of Bi/Bi₂S₃ Nanocomposites. ACS Applied Materials & Interfaces, 2017, 9, 4828-4834.	8.0	107
53	Multialloying effect on thermophysical properties of Cr₇C₃â€type carbides. Journal of the American Ceramic Society, 2017, 100, 1588-1597.	3.8	26
54	Boosting the Thermoelectric Performance of (Na,K)-Codoped Polycrystalline SnSe by Synergistic Tailoring of the Band Structure and Atomic-Scale Defect Phonon Scattering. Journal of the American Chemical Society, 2017, 139, 9714-9720.	13.7	168

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55	Effects of alloying elements such as Ti, Zr and Hf on the mechanical and thermodynamic properties of Pd-Base superalloy. Journal of Alloys and Compounds, 2017, 710, 589-599.	5.5	16
56	Mechanical properties and electronic structures of Fe-Al intermetallic. Physica B: Condensed Matter, 2017, 506, 1-11.	2.7	82
57	Microstructure and thermal properties of RETaO4 (RE = Nd, Eu, Gd, Dy, Er, Yb, Lu) as promising thermal barrier coating materials. Scripta Materialia, 2017, 126, 24-28.	5.2	144
58	Elaborating the phases and mechanical properties of multiphase alloy: Experimental two-dimensional mapping combined with theoretical calculations. Materials Characterization, 2017, 134, 347-353.	4.4	24
59	Effects of alloying element on stabilities, electronic structures, and mechanical properties of Pdâ€“based superalloys. Chinese Physics B, 2017, 26, 126202.	1.4	2
60	Pressure dependence of electronic structure and superconductivity of the MnX (Xâ€‰=â€‰N, P, As, Sb). Scientific Reports, 2016, 6, 21821.	3.3	21
61	The effects of ordered carbon vacancies on stability and thermo-mechanical properties of V8C7 compared with VC. Scientific Reports, 2016, 6, 34007.	3.3	14
62	Microstructure and thermal properties of a promising thermal barrier coating: YTaO4. Ceramics International, 2016, 42, 13876-13881.	4.8	64
63	Stability, chemical bonding behavior, elastic properties and lattice thermal conductivity of molybdenum and tungsten borides under hydrostatic pressure. Ceramics International, 2016, 42, 2117-2132.	4.8	43
64	The stability, electronic structure, elastic and metallic properties of manganese nitrides. RSC Advances, 2015, 5, 1620-1627.	3.6	59
65	Electronic structure, anisotropic elastic and thermal properties of the Î· phase Fe 6 W 6 C. Computational Materials Science, 2015, 108, 205-211.	3.0	29
66	Structure, stability, mechanical and electronic properties of Feâ€“P binary compounds by first-principles calculations. RSC Advances, 2015, 5, 81943-81956.	3.6	24
67	Elastic properties and electronic structures of CrxBy as superhard compounds. Journal of Alloys and Compounds, 2014, 610, 684-694.	5.5	49
68	First principles study the stability, mechanical and electronic properties of manganese carbides. Computational Materials Science, 2014, 87, 19-25.	3.0	53
69	Electronic structures mechanical and thermal properties of Vâ€“C binary compounds. RSC Advances, 2014, 4, 44959-44971.	3.6	62
70	Optimization of the thermophysical properties of the thermal barrier coating materials based on GA-SVR machine learning method: illustrated with ZrO2 doped DyTaO4 system. Materials Research Express, 0, , .	1.6	1