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	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
2	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
3	Highly Enhanced Thermoelectric Properties of Bi/Bi₂S₃ Nanocomposites. ACS Applied Materials & Interfaces, 2017, 9, 4828-4834.	8.0	107
4	Synthesis and thermophysical properties of RETa₃O₉ (REÂ=ÂCe, Nd, Sm, Eu, Gd,) Tj ETQq0 0 0 rgBT /Overlock 1266-1278.	3.8	93
5	Sub-1.4eV bandgap inorganic perovskite solar cells with long-term stability. Nature Communications, 2020, 11, 151.	12.8	92
6	Mechanical properties and electronic structures of Fe-Al intermetallic. Physica B: Condensed Matter, 2017, 506, 1-11.	2.7	82
7	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
8	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
9	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
10	Microstructure and thermal properties of a promising thermal barrier coating: YTaO4. Ceramics International, 2016, 42, 13876-13881.	4.8	64
11	Electronic structures mechanical and thermal properties of Vâ€“C binary compounds. RSC Advances, 2014, 4, 44959-44971.	3.6	62
12	The stability, electronic structure, elastic and metallic properties of manganese nitrides. RSC Advances, 2015, 5, 1620-1627.	3.6	59
13	First principles study the stability, mechanical and electronic properties of manganese carbides. Computational Materials Science, 2014, 87, 19-25.	3.0	53
14	Elastic properties and electronic structures of CrxBy as superhard compounds. Journal of Alloys and Compounds, 2014, 610, 684-694.	5.5	49
15	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
16	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
17	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
18	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

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19	The thermoâ€mechanical properties and ferroelastic phase transition of RENbO₄ (REÂ=ÂY, La,) Tj ETQq1 1 0.784314 rgBT	3.8	36
20	Thermodynamic properties of the Yb-Sb system predicted from first-principles calculations. Acta Materialia, 2021, 217, 117169.	7.9	34
21	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
22	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
23	Theoretical and experimental investigations of mechanical properties for polymorphous YTaO₄ceramics. Journal of the American Ceramic Society, 2019, 102, 7656-7664.	3.8	30
24	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
25	Understanding the Intrinsic P-Type Behavior and Phase Stability of Thermoelectric Î±-Mg₃Sb₂. ACS Applied Energy Materials, 2018, 1, 6600-6608.	5.1	28
26	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
27	Multialloying effect on thermophysical properties of Cr₇C₃â€type carbides. Journal of the American Ceramic Society, 2017, 100, 1588-1597.	3.8	26
28	Investigation on microstructures and thermo-physical properties of ferroelastic (Y1-xDyx)TaO4 ceramics. Materialia, 2018, 4, 478-486.	2.7	25
29	Structure, stability, mechanical and electronic properties of Feâ€“P binary compounds by first-principles calculations. RSC Advances, 2015, 5, 81943-81956.	3.6	24
30	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
31	Thermal properties of Y1â^'xMgxTaO4â^'x/2 ceramics via anion sublattice adjustment. Rare Metals, 2020, 39, 545-554.	7.1	22
32	Pressure dependence of electronic structure and superconductivity of the MnX (Xâ€‰=â€‰N, P, As, Sb). Scientific Reports, 2016, 6, 21821.	3.3	21
33	Firstâ€principles study of thermophysical properties of polymorphous YTaO₄ ceramics. Journal of the American Ceramic Society, 2021, 104, 6467-6480.	3.8	20
34	Wear Resistance Mechanism of ZTAP/HCCI Composites with a Honeycomb Structure. Metals, 2018, 8, 588.	2.3	19
35	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
36	Investigation of the thermophysical properties of (Y1-xYbx)TaO4 ceramics. Journal of the European Ceramic Society, 2020, 40, 3111-3121.	5.7	18

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37	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
38	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
39	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
40	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
41	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
42	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
43	Balance between strength and ductility of dilute Fe2B by high-throughput first-principles calculations. Ceramics International, 2021, 47, 4758-4768.	4.8	16
44	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
45	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
46	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
47	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
48	Interface transition layer interaction mechanism for ZTA_P/HCCI composites. Science and Engineering of Composite Materials, 2018, 25, 881-890.	1.4	12
49	Design of Fe2B-based ductile high temperature ceramics: First-principles calculations and experimental validation. Ceramics International, 2022, 48, 27163-27173.	4.8	11
50	The Effects of Laser Remelting on the Microstructure and Performance of Bainitic Steel. Metals, 2019, 9, 912.	2.3	10
51	The rattler effect of phonon propagation in defect-fluorite Dy3(Nb1-xTix)O7-x/2. Ceramics International, 2018, 44, 21998-22002.	4.8	9
52	An alternative approach to predict Seebeck coefficients: Application to La3â^'xTe4. Scripta Materialia, 2019, 169, 87-91.	5.2	9
53	First-principles study of pressure-induced phase transformations in thermoelectric Mg2Si. Journal of Alloys and Compounds, 2019, 773, 988-996.	5.5	9
54	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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55	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
56	Enhanced thermoelectric performance in inorganic CsSnI3 perovskite by doping with PbI2. Materials Letters, 2022, 308, 131127.	2.6	8
57	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
58	Electronic, mechanical and hydrogen storage properties of novel Mg3N2. Journal of Alloys and Compounds, 2019, 800, 8-15.	5.5	7
59	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
60	Quasiharmonic calculations of thermodynamic properties for La3â^'xTe4 system. Computational Materials Science, 2018, 142, 417-426.	3.0	6
61	Revealing the stability, elastic properties and electronic structures of Pd-V intermetallics via first principle calculations. AIP Advances, 2018, 8, .	1.3	6
62	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
63	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
64	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
65	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
66	Effects of alloying element on stabilities, electronic structures, and mechanical properties of Pdâ€“based superalloys. Chinese Physics B, 2017, 26, 126202.	1.4	2
67	Properties of Feâ€“Mnâ€“Al alloys with different Mn contents using density functional theory. Rare Metals, 2018, , 1.	7.1	1
68	Stability, electronic structure, mechanical properties and lattice thermal conductivity of FeS and FeS₂ polymorphs. Modern Physics Letters B, 2021, 35, 2150225.	1.9	1
69	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
70	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