

Xiaoyu Chong

List of Publications by Year in descending order

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67
papers

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citations

236925

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254184

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68
docs citations

68
times ranked

1589
citing authors

#	ARTICLE	IF	CITATIONS
1	Enhanced thermoelectric performance in inorganic CsSnI ₃ perovskite by doping with PbI ₂ . <i>Materials Letters</i> , 2022, 308, 131127.	2.6	8
2	Lattice stability, mechanical and thermal properties of a new class of multicomponent (Fe, Mo, W) ₆ C ₁₂ carbides with different atomic site configurations. <i>Ceramics International</i> , 2022, 48, 5107-5118.	4.8	8
3	Morphology, thermal stability, electronic structure and mechanical properties of δ -AlFeMnSi phases with varying Mn/Fe atomic ratios: Experimental studies and DFT calculations. <i>Journal of Alloys and Compounds</i> , 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. <i>Journal of Applied Physics</i> , 2022, 131, .	2.5	4
5	Design of Fe ₂ B-based ductile high temperature ceramics: First-principles calculations and experimental validation. <i>Ceramics International</i> , 2022, 48, 27163-27173.	4.8	11
6	Investigation on elastic properties and electronic structure of dilute Ir-based alloys by first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2021, 850, 156548.	5.5	18
7	Balance between strength and ductility of dilute Fe ₂ B by high-throughput first-principles calculations. <i>Ceramics International</i> , 2021, 47, 4758-4768.	4.8	16
8	Stability, electronic structure, mechanical properties and lattice thermal conductivity of FeS and FeS ₂ polymorphs. <i>Modern Physics Letters B</i> , 2021, 35, 2150225.	1.9	1
9	Numerical Optimization for the Geometric Configuration of Ceramics Perform in HCCI/ZTAP Wear-Resistant Composites Based on Actual Particle Model. <i>Nanoscale Research Letters</i> , 2021, 16, 71.	5.7	0
10	Correlation analysis of materials properties by machine learning: illustrated with stacking fault energy from first-principles calculations in dilute fcc-based alloys. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 295702.	1.8	13
11	High-entropy ferroelastic rare-earth tantalite ceramic: (Y _{0.2} Ce _{0.2} Sm _{0.2} Gd _{0.2} Dy _{0.2})TaO ₄ . <i>Journal of the American Ceramic Society</i> , 2021, 104, 5873-5882.		49
12	Probing the mechanical properties of ordered and disordered Pt-Ir alloys by first-principles calculations. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2021, 405, 127424.	2.1	17
13	First-principles study of thermophysical properties of polymorphous YTaO ₄ ceramics. <i>Journal of the American Ceramic Society</i> , 2021, 104, 6467-6480.	3.8	20
14	Exploring crystal structures, stability and mechanical properties of Fe, Mn-containing intermetallics in Al-Si Alloy by experiments and first-principles calculations. <i>Journal of Alloys and Compounds</i> , 2021, 876, 160022.	5.5	28
15	Thermodynamic properties of the Yb-Sb system predicted from first-principles calculations. <i>Acta Materialia</i> , 2021, 217, 117169.	7.9	34
16	First-Principles Calculations of Thermal and Electrical Transport Properties of bcc and fcc Dilute Fe-X (X = Al, Co, Cr, Mn, Mo, Nb, Ni, Ti, V, and W) Binary Alloys. <i>Metals</i> , 2021, 11, 1988.	2.3	6
17	Sub-1.4eV bandgap inorganic perovskite solar cells with long-term stability. <i>Nature Communications</i> , 2020, 11, 151.	12.8	92
18	The thermo-mechanical properties and ferroelastic phase transition of RENbO ₄ (RE = Y, La). <i>Tj ETQg 0.0 0 rgBT /Overlock</i>	3.8	36

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19	Effects of the alloying element on the stacking fault energies of dilute Ir-based superalloys: A comprehensive first-principles study. <i>Journal of Materials Research</i> , 2020, 35, 2718-2725.	2.6	7
20	Anisotropic mechanical properties and electronic structures of transition metal carbonitrides M ₂ CN (M = V, Ti, Ta, Nb, Hf and Zr) by first-principles calculations. <i>Applied Physics A: Materials Science and Processing</i> , 2020, 126, 1.	2.3	4
21	The investigation on structural, electronic, elastic, adsorptive, catalytic and magnetic properties of precious metal materials via first-principles calculations based on density functional theory – a review. <i>Journal of Micromechanics and Molecular Physics</i> , 2020, 05, 2030001.	1.2	9
22	Effect of solution treatment on mechanical properties and microstructure of welded joints of Fe-29Mn-9Al-0.9C low-density steel. <i>Journal of Micromechanics and Molecular Physics</i> , 2020, 05, 2050006.	1.2	6
23	Investigation of the thermophysical properties of (Y _{1-x} Y _b)TaO ₄ ceramics. <i>Journal of the European Ceramic Society</i> , 2020, 40, 3111-3121.	5.7	18
24	Mechanical and thermal properties of RE ₂ TaO ₄ (RE = Yb, Lu, Sc) ceramics with monoclinic-prime phase. <i>Journal of Materials Science and Technology</i> , 2020, 52, 20-28.	10.7	40
25	Investigation on the stability, electronic, optical, and mechanical properties of novel calcium carbonate hydrates via first-principles calculations. <i>International Journal of Quantum Chemistry</i> , 2020, 120, e26219.	2.0	8
26	Achieving a fine balance in mechanical properties and thermoelectric performance in commercial Bi ₂ Te ₃ materials. <i>Ceramics International</i> , 2020, 46, 14994-15002.	4.8	34
27	Thermodynamic analysis of the interface reaction and thermal stress of WCp/Fe composites. <i>Ceramics International</i> , 2020, 46, 26210-26215.	4.8	11
28	Rapid screening of alloy elements to improve the elastic properties of dilute Pt-based alloys: High-throughput first-principles calculations and modeling. <i>Journal of Applied Physics</i> , 2020, 128, .	2.5	16
29	The effect of ZrO ₂ alloying on the microstructures and thermal properties of DyTaO ₄ for high-temperature application. <i>Journal of the American Ceramic Society</i> , 2019, 102, 889-895.	3.8	16
30	Temperature and stress field analysis of solidification process in high chromium cast iron matrix composite reinforced by ZTA ceramic particles. <i>Materials Research Express</i> , 2019, 6, 106551.	1.6	5
31	The Effects of Laser Remelting on the Microstructure and Performance of Bainitic Steel. <i>Metals</i> , 2019, 9, 912.	2.3	10
32	An alternative approach to predict Seebeck coefficients: Application to La _{3-x} Te ₄ . <i>Scripta Materialia</i> , 2019, 169, 87-91.	5.2	9
33	Theoretical and experimental investigations of mechanical properties for polymorphous YTaO ₄ ceramics. <i>Journal of the American Ceramic Society</i> , 2019, 102, 7656-7664.	3.8	30
34	Multipoint Defect Synergy Realizing the Excellent Thermoelectric Performance of n-Type Polycrystalline SnSe via Re Doping. <i>Advanced Functional Materials</i> , 2019, 29, 1902893.	14.9	73
35	Tailoring the anisotropic mechanical properties of hexagonal M ₇ X ₃ (M=Fe, Cr, W, Mo; X=C, B) by multialloying. <i>Acta Materialia</i> , 2019, 169, 193-208.	7.9	74
36	Stability, mechanical and electronic properties of ceramic interphases in biomedical composites via first-principles calculations. <i>Ceramics International</i> , 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. <i>Journal of Alloys and Compounds</i> , 2018, 745, 196-211.	5.5	32
38	Effect of Al ³⁺ doping on mechanical and thermal properties of DyTaO ₄ as promising thermal barrier coating application. <i>Journal of the American Ceramic Society</i> , 2018, 101, 1818-1823.	3.8	32
39	Synthesis and thermophysical properties of RETa ₃ O ₉ (RE = Ce, Nd, Sm, Eu, Gd). <i>Journal of Alloys and Compounds</i> , 2018, 745, 1266-1278.	3.8	93
40	Enhanced thermoelectric properties of bismuth telluride bulk achieved by telluride-spilling during the spark plasma sintering process. <i>Scripta Materialia</i> , 2018, 143, 90-93.	5.2	77
41	Quasiharmonic calculations of thermodynamic properties for La ₃ Te ₄ system. <i>Computational Materials Science</i> , 2018, 142, 417-426.	3.0	6
42	A first-principles calculation of structural, mechanical, thermodynamic and electronic properties of binary Ni ²⁺ Y compounds. <i>RSC Advances</i> , 2018, 8, 41575-41586.	3.6	17
43	Investigation on microstructures and thermo-physical properties of ferroelastic (Y _{1-x} Dy _x)TaO ₄ ceramics. <i>Materialia</i> , 2018, 4, 478-486.	2.7	25
44	Revealing the stability, elastic properties and electronic structures of Pd-V intermetallics via first principle calculations. <i>AIP Advances</i> , 2018, 8, .	1.3	6
45	Understanding the Intrinsic P-Type Behavior and Phase Stability of Thermoelectric Mg_3Sb_2 . <i>ACS Applied Energy Materials</i> , 2018, 1, 6600-6608.	5.1	28
46	Wear Resistance Mechanism of ZTAP/HCCI Composites with a Honeycomb Structure. <i>Metals</i> , 2018, 8, 588.	2.3	19
47	The rattler effect of phonon propagation in defect-fluorite Dy ₃ (Nb _{1-x} Ti _x)O _{7-x/2} . <i>Ceramics International</i> , 2018, 44, 21998-22002.	4.8	9
48	Achieving high thermoelectric performance of Cu _{1.8} S composites with WSe ₂ nanoparticles. <i>Nanotechnology</i> , 2018, 29, 345402.	2.6	19
49	Exploring accurate structure, composition and thermophysical properties of δ -carbides in 17.90 wt% W-4.15 wt% Cr-1.10 wt% V-0.69 wt% C steel. <i>Scripta Materialia</i> , 2018, 154, 149-153.	5.2	18
50	Multialloying effect on thermophysical properties of Cr ₇ C ₃ -type carbides. <i>Journal of the American Ceramic Society</i> , 2017, 100, 1588-1597.	3.8	26
51	Boosting the Thermoelectric Performance of (Na,K)-Codoped Polycrystalline SnSe by Synergistic Tailoring of the Band Structure and Atomic-Scale Defect Phonon Scattering. <i>Journal of the American Chemical Society</i> , 2017, 139, 9714-9720.	13.7	168
52	Effects of alloying elements such as Ti, Zr and Hf on the mechanical and thermodynamic properties of Pd-Base superalloy. <i>Journal of Alloys and Compounds</i> , 2017, 710, 589-599.	5.5	16
53	Mechanical properties and electronic structures of Fe-Al intermetallic. <i>Physica B: Condensed Matter</i> , 2017, 506, 1-11.	2.7	82
54	Microstructure and thermal properties of RETaO ₄ (RE = Nd, Eu, Gd, Dy, Er, Yb, Lu) as promising thermal barrier coating materials. <i>Scripta Materialia</i> , 2017, 126, 24-28.	5.2	144

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55	Stability, electronic structure, mechanical and thermodynamic properties of Fe-Si binary compounds. Journal of Alloys and Compounds, 2017, 693, 859-870.	5.5	41
56	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
57	Pressure dependence of electronic structure and superconductivity of the MnX (X=As, N, P, As, Sb). Scientific Reports, 2016, 6, 21821.	3.3	21
58	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
59	Microstructure and thermal properties of a promising thermal barrier coating: YTaO4. Ceramics International, 2016, 42, 13876-13881.	4.8	64
60	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
61	Numerical simulation of mold filling process for high chromium cast iron matrix composite reinforced by ZTA ceramic particles. International Journal of Heat and Mass Transfer, 2015, 89, 872-883.	4.8	27
62	Electronic structure, anisotropic elastic and thermal properties of the $\hat{\Gamma}$ -phase Fe ₆ W ₆ C. Computational Materials Science, 2015, 108, 205-211.	3.0	29
63	Structure, stability, mechanical and electronic properties of Fe-P binary compounds by first-principles calculations. RSC Advances, 2015, 5, 81943-81956.	3.6	24
64	Elastic properties and electronic structures of Cr _x B _y as superhard compounds. Journal of Alloys and Compounds, 2014, 610, 684-694.	5.5	49
65	First principles study the stability, mechanical and electronic properties of manganese carbides. Computational Materials Science, 2014, 87, 19-25.	3.0	53
66	Electronic structures mechanical and thermal properties of V-C binary compounds. RSC Advances, 2014, 4, 44959-44971.	3.6	62
67	Optimization of the thermophysical properties of the thermal barrier coating materials based on GA-SVR machine learning method: illustrated with ZrO ₂ doped DyTaO ₄ system. Materials Research Express, 0, .	1.6	1