William Yi Wang

List of Publications by Year
in descending order

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107	2,878	172207	214527
papers	citations	29 h-index	47 g-index

109	109	109	2424
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Generalized stacking fault energy, ideal strength and twinnability of dilute Mg-based alloys: A first-principles study of shear deformation. Acta Materialia, 2014, 67, 168-180.	3.8	193
2	A mixed-space approach to first-principles calculations of phonon frequencies for polar materials. Journal of Physics Condensed Matter, 2010, 22, 202201.	0.7	167
3	A comprehensive first-principles study of pure elements: Vacancy formation and migration energies and self-diffusion coefficients. Acta Materialia, 2016, 109, 128-141.	3.8	117
4	Effects of Alloying Elements on Stacking Fault Energies and Electronic Structures of Binary Mg Alloys: A First-Principles Study. Materials Research Letters, 2014, 2, 29-36.	4.1	95
5	Integrating data mining and machine learning to discover high-strength ductile titanium alloys. Acta Materialia, 2021, 202, 211-221.	3.8	85
6	Integrated computational materials engineering for advanced materials: A brief review. Computational Materials Science, 2019, 158, 42-48.	1.4	84
7	Evading the strength-ductility trade-off at room temperature and achieving ultrahigh plasticity at 800â„ƒ in a TiAl alloy. Acta Materialia, 2022, 225, 117585.	3.8	75
8	Microstructure and properties of bulk Al0.5CoCrFeNi high-entropy alloy by cold rolling and subsequent annealing. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2018, 729, 141-148.	2.6	74
9	Phase stability and mechanical properties of AlHfNbTiZr high-entropy alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2018, 724, 249-259.	2.6	67
10	Fabrication and Characterization of Beaded SiC Quantum Rings with Anomalous Red Spectral Shift. Advanced Materials, 2012, 24, 5598-5603.	11.1	65
11	Temperature-dependent ideal strength and stacking fault energy of fcc Ni: a first-principles study of shear deformation. Journal of Physics Condensed Matter, 2012, 24, 155402.	0.7	64
12	Atomic and electronic basis for the serrations of refractory high-entropy alloys. Npj Computational Materials, 2017, 3, .	3.5	64
13	Anomalous structural dynamics in liquid Al80Cu20: An ab initio molecular dynamics study. Acta Materialia, 2015, 97, 75-85.	3.8	62
14	Computation of entropies and phase equilibria in refractory V-Nb-Mo-Ta-W high-entropy alloys. Acta Materialia, 2018, 143, 88-101.	3.8	55
15	Predicting densities and elastic moduli of SiO2-based glasses by machine learning. Npj Computational Materials, 2020, 6, .	3.5	52
16	Nanophase precipitation and strengthening in a dual-phase Al0.5CoCrFeNi high-entropy alloy. Journal of Materials Science and Technology, 2021, 72, 1-7.	5.6	51
17	High strength Mg-Zn-Y alloys reinforced synergistically by Mg12ZnY phase and Mg3Zn3Y2 particle. Journal of Alloys and Compounds, 2017, 703, 508-516.	2.8	50
18	High-Throughput Calculations for High-Entropy Alloys: A Brief Review. Frontiers in Materials, 2020, 7, .	1.2	50

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19	Local lattice distortion mediated formation of stacking faults in Mg alloys. Acta Materialia, 2019, 170, 231-239.	3.8	45
20	Electronic structures of long periodic stacking order structures in Mg: A first-principles study. Journal of Alloys and Compounds, 2014, 586, 656-662.	2.8	42
21	Disorder in Mn+1AXn phases at the atomic scale. Nature Communications, 2019, 10, 622.	5.8	41
22	Atomic and electronic basis for solutes strengthened (010) anti-phase boundary of L12 Co3(Al, TM): A comprehensive first-principles study. Acta Materialia, 2018, 145, 30-40.	3.8	40
23	Atomic structure and diffusivity in liquid Al80Ni20 by ab initio molecular dynamics simulations. Physica B: Condensed Matter, 2011, 406, 3089-3097.	1.3	38
24	Electron localization morphology of the stacking faults in Mg: A first-principles study. Chemical Physics Letters, 2012, 551, 121-125.	1.2	37
25	stretchy="false">[</mml:mo><mml:mn>1</mml:mn><mml:mover accent="true"><mml:mrow><mml:mn>1</mml:mn></mml:mrow><mml:mrow><mml:mo>-</mml:mo></mml:mrow></mml:mover><mml:mo	1.4	37
26	Effect of strong magnetic field on the microstructure and mechanical-magnetic properties of AlCoCrFeNi high-entropy alloy. Journal of Alloys and Compounds, 2020, 820, 153407.	2.8	34
27	Tailoring mechanical and magnetic properties of AlCoCrFeNi high-entropy alloy via phase transformation. Journal of Materials Science and Technology, 2021, 73, 83-90.	5.6	34
28	Insight into structural, elastic, phonon, and thermodynamic properties of Î±-sulfur and energy-related sulfides: a comprehensive first-principles study. Journal of Materials Chemistry A, 2015, 3, 8002-8014.	5.2	33
29	Liquid-phase separation in undercooled CoCrCuFeNi high entropy alloy. Intermetallics, 2017, 86, 110-115.	1.8	30
30	Anomalous phonon stiffening associated with the (1 1 1) antiphase boundary in L12 Ni3Al. Acta Materialia, 2015, 82, 287-294.	3.8	29
31	Revealing the local lattice strains and strengthening mechanisms of Ti alloys. Computational Materials Science, 2018, 152, 169-177.	1.4	29
32	Electrocarving during Electrodeposition Growth. Advanced Materials, 2018, 30, e1805686.	11.1	28
33	Optimizing mechanical and magnetic properties of AlCoCrFeNi high-entropy alloy via FCC to BCC phase transformation. Journal of Materials Science and Technology, 2021, 86, 117-126.	5.6	27
34	Cr-based bulk metallic glasses with ultrahigh hardness. Applied Physics Letters, 2015, 106, .	1.5	26
35	Evolution of microstructure and hardness in a dual-phase Al0.5CoCrFeNi high-entropy alloy with different grain sizes. Rare Metals, 2020, 39, 156-161.	3.6	25
36	Effect of solute atoms on glass-forming ability for Feâ€“Yâ€“B alloy: An ab initio molecular dynamics study. Acta Materialia, 2014, 77, 96-110.	3.8	24

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37	Power law scaled hardness of Mn strengthened nanocrystalline Al Mn non-equilibrium solid solutions. Scripta Materialia, 2016, 120, 31-36.	2.6	24
38	Composition dependence of diffusion and thermotransport in Ni-Al melts: A step towards molecular dynamics assisted databases. Acta Materialia, 2017, 136, 74-89.	3.8	24
39	Fully Recrystallized Al0.5CoCrFeNi High-Entropy Alloy Strengthened by Nanoscale Precipitates. Metals and Materials International, 2019, 25, 1145-1150.	1.8	24
40	Bonding charge density from atomic perturbations. Journal of Computational Chemistry, 2015, 36, 1008-1014.	1.5	23
41	First-principles investigation of phase stability, elastic and thermodynamic properties in L12 Co3(Al,Mo,Nb) phase. Intermetallics, 2016, 78, 1-7.	1.8	22
42	Temperature dependent deformation mechanisms of Al0.3CoCrFeNi high-entropy alloy, starting from serrated flow behavior. Journal of Alloys and Compounds, 2018, 757, 39-43.	2.8	22
43	Effects of Composition on Atomic Structure, Diffusivity, and Viscosity of Liquid Al-Zr Alloys. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2012, 43, 3471-3480.	1.1	21
44	Revealing the Microstates of Body-Centered-Cubic (BCC) Equiatomic High Entropy Alloys. Journal of Phase Equilibria and Diffusion, 2017, 38, 404-415.	0.5	21
45	Elastic properties of long periodic stacking ordered phases in Mg-Gd-Al alloys: A first-principles study. Intermetallics, 2018, 98, 18-27.	1.8	21
46	Effects of reactive elements on the structure and diffusivity of liquid chromia: Anab initiomolecular dynamics study. Physical Review B, 2012, 85, .	1.1	19
47	Local electronic descriptors for solute-defect interactions in bcc refractory metals. Nature Communications, 2019, 10, 4484.	5.8	19
48	High strength Mg 94 Zn 2.4 Y 3.6 alloy with long period stacking ordered structure prepared by near-rapid solidification technology. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2017, 679, 476-483.	2.6	18
49	Coupling effects of high magnetic field and annealing on the microstructure evolution and mechanical properties of additive manufactured Tiâ€“6Alâ€“4V. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2021, 824, 141815.	2.6	18
50	Solid-Solution Hardening in Mg-Gd-TM (TMÂ=ÂAg, Zn, and Zr) Alloys: An Integrated Density Functional Theory and Electron Work Function Study. Jom, 2015, 67, 2433-2441.	0.9	17
51	Lattice distortion induced anomalous ferromagnetism and electronic structure in FCC Fe and Fe-TM (TMÂ=ÂCr, Ni, Ta and Zr) alloys. Materials Chemistry and Physics, 2015, 162, 748-756.	2.0	17
52	Strengthening Mg by self-dispersed nano-lamellar faults. Materials Research Letters, 2017, 5, 415-425.	4.1	17
53	Insight into solid-solution strengthened bulk and stacking faults properties in Ti alloys: a comprehensive first-principles study. Journal of Materials Science, 2018, 53, 7493-7505.	1.7	17
54	A brief review of data-driven ICME for intelligently discovering advanced structural metal materials: Insight into atomic and electronic building blocks. Journal of Materials Research, 2020, 35, 872-889.	1.2	17

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55	Hot Deformation and Subsequent Annealing on the Microstructure and Hardness of an Al0.3CoCrFeNi High-entropy Alloy. Acta Metallurgica Sinica (English Letters), 2021, 34, 1527-1536.	1.5	17
56	Structure and energetics of Ni from ab initio molecular dynamics calculations. Computational Materials Science, 2014, 89, 242-246.	1.4	16
57	Formation of a hexagonal closed-packed phase in Al0.5CoCrFeNi high entropy alloy. MRS Communications, 2017, 7, 879-884.	0.8	16
58	When a defect is a pathway to improve stability: a case study of the L12 Co3TM superlattice intrinsic stacking fault. Journal of Materials Science, 2019, 54, 13609-13618.	1.7	16
59	Metadynamic recrystallization behavior of Î²-solidified TiAl alloy during post-annealing after hot deformation. Intermetallics, 2020, 117, 106679.	1.8	15
60	Revealing foundations of the intergranular corrosion of 5XXX and 6XXX Al alloys. Materials Letters, 2020, 271, 127767.	1.3	15
61	Electronic structures and properties of TiAl/Ti2AlNb heterogeneous interfaces: A comprehensive first-principles study. Intermetallics, 2021, 133, 107173.	1.8	15
62	Origin of enhanced glass-forming ability of Ce-containing Alâ€“Fe alloy: Ab initio molecular dynamics study. Intermetallics, 2014, 46, 29-39.	1.8	14
63	Tensile properties and deformation micromechanism of Ti-based metallic glass composite containing impurity elements. Journal of Alloys and Compounds, 2019, 784, 220-230.	2.8	14
64	Irradiationâ€Induced Extremes Create Hierarchical Faceâ€/Bodyâ€Centeredâ€Cubic Phases in Nanostructured High Entropy Alloys. Advanced Materials, 2020, 32, 2002652.	11.1	14
65	High-throughput investigations of configurational-transformation-dominated serrations in CuZr/Cu nanolaminates. Journal of Materials Science and Technology, 2020, 53, 192-199.	5.6	14
66	Formation mechanism of Î³ twins in Î²-solidified Î³-TiAl alloys. Journal of Materials Science and Technology, 2022, 105, 164-171.	5.6	14
67	Effect of Cold Rolling on the Phase Transformation Kinetics of an Al0.5CoCrFeNi High-Entropy Alloy. Entropy, 2018, 20, 917.	1.1	13
68	Phase Stability and Deformation Behavior of TiZrHfNbO High-Entropy Alloys. Frontiers in Materials, 2020, 7, .	1.2	13
69	Structural mechanism for ultrahigh-strength Co-based metallic glasses. Scripta Materialia, 2013, 68, 257-260.	2.6	12
70	Influence of the interatomic potential on thermotransport in binary liquid alloys: case study on NiAl. Philosophical Magazine, 2016, 96, 3054-3074.	0.7	12
71	Circumventing silver oxidation induced performance degradation of silver surface-enhanced Raman scattering substrates. Nanotechnology, 2018, 29, 414001.	1.3	12
72	Robust Superlubricity and MoirÃ© Latticeâ€™s Size Dependence on Friction between Graphdiyne Layers. ACS Applied Materials & Interfaces, 2021, 13, 40901-40908.	4.0	12

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73	Impact of W on structural evolution and diffusivity of Niâ€“W melts: an ab initio molecular dynamics study. Journal of Materials Science, 2015, 50, 1071-1081.	1.7	11
74	Nano-sized Superlattice Clusters Created by Oxygen Ordering in Mechanically Alloyed Fe Alloys. Scientific Reports, 2015, 5, 11772.	1.6	11
75	Interdiffusion and thermotransport in Niâ€“Al liquid alloys. Philosophical Magazine, 2018, 98, 2221-2246.	0.7	11
76	Accurate determination of thermodynamic properties for liquid alloys based on ab initio molecular dynamics simulation. Fluid Phase Equilibria, 2013, 360, 44-53.	1.4	10
77	Prediction of Diffusion Coefficients in Liquid and Solids. Defect and Diffusion Forum, 0, 364, 182-191.	0.4	10
78	First-principles calculations of lattice dynamics and thermodynamic properties for Yb14MnSb11. Journal of Applied Physics, 2018, 123, .	1.1	10
79	Mass and thermal transport in liquid Cu-Ag alloys. Philosophical Magazine, 2019, 99, 468-491.	0.7	10
80	Hot deformation study and interface characterization for TiAl/Ti2AlNb diffusion bonds based on the serial constitutive model. Intermetallics, 2019, 104, 66-73.	1.8	10
81	Experimental and simulation analysis of residual topography dominated deformation mechanism of nanoindentation: a case study of Inconel 625 superalloy. Journal of Materials Research and Technology, 2021, 13, 1521-1533.	2.6	10
82	Low energy structures of lithium-ion battery materials Li(MnxNixCo1â^'2x)O2 revealed by first-principles calculations. Applied Physics Letters, 2013, 103, .	1.5	9
83	Combined crystal plasticity simulations and experiments for parameter identification: application to near-Î² titanium alloy. Journal of Materials Science, 2020, 55, 15043-15055.	1.7	9
84	Interstitial triggered grain boundary embrittlement of Alâ€“X (Xâ€¯=â€¯H, N and O). Computational Materials Science, 2019, 163, 241-247.	1.4	8
85	Thermalâ€“Mechanical Processing and Strengthen in AlxCoCrFeNi High-Entropy Alloys. Frontiers in Materials, 2021, 7, .	1.2	8
86	Local orders, lattice distortions, and electronic structure dominated mechanical properties of (ZrHfTaM1M2)C (M = Nb, Ti, V). Journal of the American Ceramic Society, 2022, 105, 4260-4276.	1.9	8
87	Pitting Corrosion of Natural Aged Alâ€“Mgâ€“Si Extrusion Profile. Materials, 2019, 12, 1081.	1.3	7
88	A new microscopic coordinated deformation model of Ti-based bulk metallic composites during tensile deformation. Scripta Materialia, 2019, 172, 23-27.	2.6	6
89	Lattice distortion-enhanced superlubricity of (Mo, X)S₂ (X = Al, Ti, Cr and V) with moirÃ© superlattice. Nanoscale, 2021, 13, 16234-16243.	2.8	6
90	Experiments and crystal plasticity simulations for the deformation behavior of nanoindentation: Application to the Î±2 phase of TiAl alloy. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2021, 831, 142283.	2.6	6

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91	Activation volume dominated diffusivity of Ni50Al50 melt under extreme conditions. Computational Materials Science, 2020, 171, 109263.	1.4	5
92	Improved Mechanical Properties of Additive Manufactured Ti-6Al-4V Alloy via Annealing in High Magnetic Field. Rare Metal Materials and Engineering, 2018, 47, 3678-3685.	0.8	4
93	DID Code: A Bridge Connecting the Materials Genome Engineering Database with Inheritable Integrated Intelligent Manufacturing. Engineering, 2020, 6, 612-620.	3.2	4
94	Revealing sulfur- and phosphorus-induced embrittlement and local structural phase transformation of superlattice intrinsic stacking faults in L12-Ni3Al. Journal of Materials Science, 2022, 57, 12483-12496.	1.7	4
95	High strength Mgâ€“Znâ€“Y alloys reinforced synergistically by Nano-SiCp and long period stacking ordered structure. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2019, 765, 138284.	2.6	3
96	Computer simulation of thermodynamic factors in Ni-Al and Cu-Ag liquid alloys. Computational Materials Science, 2019, 166, 124-135.	1.4	3
97	Effect of High Strain Rate on Adiabatic Shearing of Î±+Î² Dual-Phase Ti Alloy. Materials, 2021, 14, 2044.	1.3	3
98	Site Occupation and Structural Phase Transformation of the (010) Antiphase Boundary in Boron-Modified L12 Ni3Al. Jom, 2021, 73, 2285-2292.	0.9	2
99	Revealing the Local Microstates of Feâ€“Mnâ€“Al Medium Entropy Alloy: A Comprehensive First-principles Study. Acta Metallurgica Sinica (English Letters), 2021, 34, 1492-1502.	1.5	2
100	The Localized Corrosion and Stress Corrosion Cracking of a 6005A-T6 Extrusion Profile. Materials, 2021, 14, 4924.	1.3	1
101	Locking of Screw Dislocations in Silicon due to Core Structure Transformation. Journal of Physical Chemistry C, 2021, 125, 24710-24718.	1.5	1
102	Effect of High Strain Rates on Adiabatic Shear Bands Evolution and Mechanical Performance of Dual-Phase Ti Alloy. Frontiers in Materials, 2022, 8, .	1.2	1
103	Local Lattice Distortion Mediated Formation of Stacking Faults in Mg Alloys. SSRN Electronic Journal, 0, , .	0.4	0
104	Editorial: Data-Driven Integrated Computational Materials Engineering for High-Entropy Materials. Frontiers in Materials, 2021, 8, .	1.2	0
105	Kinetics and Thermodynamics of Fe-X (X= Al, Cr, Mn, Ti, B, and C) Melts under High Pressure. , 0, 29, 143-160.		0
106	Solid Solution Hardening in Mg-Gd-TM (TM=Ag, Zn and Zr) Alloys: An Integrated Density Functional Theory and Electron Work Function Study. , 2016, , 157-157.		0
107	Highâ€Entropy Alloys: Irradiationâ€Induced Extremes Create Hierarchical Faceâ€/Bodyâ€Centeredâ€Cubic Phases in Nanostructured High Entropy Alloys (Adv. Mater. 39/2020). Advanced Materials, 2020, 32, .	11.1	0