Chao Jiang

List of Publications by Year
in descending order

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113 papers	5,422 citations	76326 40 h-index	85541 71 g-index
113 all docs	113 docs citations	113 times ranked	5118 citing authors

#	Article	IF	Citations
1	Freestanding Nanostructures via Layer-by-Layer Assembly. Advanced Materials, 2006, 18, 829-840.	21.0	387
2	Ab initio lattice stability in comparison with CALPHAD lattice stability. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2004, 28, 79-90.	1.6	340
3	Band-gap engineering for removing shallow traps in rare-earth Lu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>Al<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>5</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /></mml:msub></mml:math>	3.2	288
4	First-principles study of binary bcc alloys using special quasirandom structures. Physical Review B, 2004, 69, .	3.2	266
5	Compliant, Robust, and Truly Nanoscale Free-Standing Multilayer Films Fabricated Using Spin-Assisted Layer-by-Layer Assembly. Advanced Materials, 2004, 16, 157-161.	21.0	221
6	Freely Suspended Layer-by-Layer Nanomembranes: Testing Micromechanical Properties. Advanced Functional Materials, 2005, 15, 771-780.	14.9	182
7	First-principles prediction of disordering tendencies in pyrochlore oxides. Physical Review B, 2009, 79, .	3.2	140
8	Structural, elastic, and electronic properties of Fe3C from first principles. Journal of Applied Physics, 2008, 103, .	2.5	134
9	Site preference of transition metal elements in Ni3Al. Scripta Materialia, 2006, 55, 433-436.	5.2	133
10	Site preference of ternary alloying elements in Ni3Al: A first-principles study. Acta Materialia, 2006, 54, 1147-1154.	7.9	130
11	First-principles study of structural, elastic, and electronic properties of chromium carbides. Applied Physics Letters, 2008, 92, .	3.3	116
12	EfficientAbÂinitioModeling of Random Multicomponent Alloys. Physical Review Letters, 2016, 116, 105501.	7.8	93
13	Thermodynamic properties of the Alâ€“Feâ€“Ni system acquired via a hybrid approach combining calorimetry, first-principles and CALPHAD. Acta Materialia, 2009, 57, 5324-5341.	7.9	90
14	Deviations from Vegardâ€™s law in ternary III-V alloys. Physical Review B, 2010, 82, .	3.2	89
15	First-principles study of Co3(Al,W) alloys using special quasi-random structures. Scripta Materialia, 2008, 59, 1075-1078.	5.2	85
16	Role of Antisite Disorder on Preamorphization Swelling in Titanate Pyrochlores. Physical Review Letters, 2012, 108, 195504.	7.8	85
17	Site preference of transition-metal elements in B2 NiAl: A comprehensive study. Acta Materialia, 2007, 55, 4799-4806.	7.9	78
18	Freely Suspended Gold Nanoparticle Arrays. Advanced Materials, 2005, 17, 1669-1673.	21.0	74

#	Article	IF	Citations
19	A combined first-principles and experimental study of the lattice site preference of Pt in B2 NiAl. Acta Materialia, 2005, 53, 2101-2109.	7.9	71
20	Pressure-Induced Cubic to Monoclinic Phase Transformation in Erbium Sesquioxide Er2O3. Inorganic Chemistry, 2007, 46, 6164-6169.	4.0	71
21	Thermodynamic and Mechanical Stabilities of Tantalum Nitride. Physical Review Letters, 2009, 103, 185501.	7.8	68
22	First-principles calculations and thermodynamic modeling of the Niâ€“Mo system. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2005, 397, 288-296.	5.6	67
23	First-principles study of ternary bcc alloys using special quasi-random structures. Acta Materialia, 2009, 57, 4716-4726.	7.9	66
24	Defect interactions in Sn1âˆ’xGex random alloys. Applied Physics Letters, 2009, 94, 252104.	3.3	65
25	E centers in ternary Si1âˆ’xâˆ’yGexSny random alloys. Applied Physics Letters, 2009, 95, .	3.3	64
26	Effects of Cu and Al on the crystal structure and composition of Î· (MgZn2) phase in over-aged Alâ€“Znâ€“Mgâ€“Cu alloys. Journal of Materials Science, 2012, 47, 5419-5427.	3.7	64
27	Unexpected strain-stiffening in crystalline solids. Nature, 2013, 496, 339-342.	27.8	64
28	Nonlinear stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>E</mml:mi></mml:math>centers in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Si</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn> Electronic structure calculations. Physical Review B, 2008, 78, .	3.2	63
29	Band-Gap and Band-Edge Engineering of Multicomponent Garnet Scintillators from First Principles. Physical Review Applied, 2015, 4, .	3.8	62
30	Opposite correlations between cation disordering and amorphization resistance in spinels versus pyrochlores. Nature Communications, 2015, 6, 8750.	12.8	62
31	Strain-Sensitive Raman Modes of Carbon Nanotubes in Deflecting Freely Suspended Nanomembranes. Advanced Materials, 2005, 17, 2127-2131.	21.0	61
32	Flexible and Robust 2D Arrays of Silver Nanowires Encapsulated within Freestanding Layer-by-Layer Films. Advanced Functional Materials, 2006, 16, 2024-2034.	14.9	61
33	Phase transformation in Sm2O3 at high pressure: In situ synchrotron X-ray diffraction study and ab initio DFT calculation. Solid State Communications, 2008, 145, 250-254.	1.9	59
34	Predicted structure and stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>A</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:msub><mml:mi>B</mml:mi><mml:m xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î´</mml:mi></mml:math>-phase compositions. Physical Review B, 2009, 80, .	3.2	54
35	Effect of Grain Boundary Stresses on Sink Strength. Materials Research Letters, 2014, 2, 100-106.	8.7	51
36	First-principles study of site occupancy of dilute 3d, 4d and 5d transition metal solutes in L10 TiAl. Acta Materialia, 2008, 56, 6224-6231.	7.9	49

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37	Site preference of early transition metal elements in C15 NbCr2. Acta Materialia, 2007, 55, 1599-1605.	7.9	47
38	Nuclear wasteform materials: Atomistic simulation case studies. Journal of Nuclear Materials, 2013, 441, 29-39.	2.7	45
39	First-principles study of constitutional point defects in B2 NiAl using special quasirandom structures. Acta Materialia, 2005, 53, 2643-2652.	7.9	42
40	First-principles prediction of mechanical properties of gamma-boron. Applied Physics Letters, 2009, 94, 191906.	3.3	40
41	Formation and self-organization of void superlattices under irradiation: A phase field study. Materialia, 2018, 1, 78-88.	2.7	39
42	First-principles study of phase stability in pseudobinary(Ni1â^'xPtx)3Alalloys. Physical Review B, 2005, 72, .	3.2	38
43	Amorphization Driven by Defect-Induced Mechanical Instability. Physical Review Letters, 2013, 111, 155501.	7.8	35
44	Effects of Cu content on the precipitation process of Alâ€"Znâ€"Mg alloys. Journal of Materials Science, 2012, 47, 8174-8187.	3.7	34
45	Carbon tri-interstitial defect: A model for the D<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>II</mml:mi></mml:msub></mml:math>center. Physical Review B, 2012, 86, .	3.2	33
46	Anisotropic hydrogen diffusion in Î±-Zr and Zircaloy predicted by accelerated kinetic Monte Carlo simulations. Scientific Reports, 2017, 7, 41033.	3.3	33
47	Using Machine Learning To Identify Factors That Govern Amorphization of Irradiated Pyrochlores. Chemistry of Materials, 2017, 29, 2574-2583.	6.7	33
48	Freestanding 2D Arrays of Silver Nanorods. Advanced Materials, 2006, 18, 2895-2899.	21.0	32
49	Effects of Pt on the elastic properties of B2 NiAl: A combined first-principles and experimental study. Acta Materialia, 2006, 54, 2361-2369.	7.9	30
50	Trilayered Ceramicâ€"Metalâ€"Polymer Microcantilevers with Dramatically Enhanced Thermal Sensitivity. Advanced Materials, 2006, 18, 1157-1161.	21.0	29
51	The effect of Gaâ€doping on the defect chemistry of RE₃Al₅O₁₂ garnets. Physica Status Solidi (B): Basic Research, 2013, 250, 244-248.	1.5	29
52	First-principles based modeling of hydrogen permeation through Pdâ€"Cu alloys. International Journal of Hydrogen Energy, 2012, 37, 12760-12764.	7.1	28
53	Theoretical prediction and atomic kinetic Monte Carlo simulations of void superlattice self-organization under irradiation. Scientific Reports, 2018, 8, 6629.	3.3	27
54	Point defect thermodynamics and diffusion in Fe3C: A first-principles study. Acta Materialia, 2008, 56, 3236-3244.	7.9	26

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55	Native defects and the arsenic vacancy defect in In<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>As. Physical Review B, 2011, 84, .	3.2	26
56	A first-principles study of the site preference of Cr in B2 NiAl. Scripta Materialia, 2006, 54, 405-410.	5.2	25
57	Predicting from first principles the chemical evolution of crystalline compounds due to radioactive decay: The case of the transformation of CsCl to BaCl. Physical Review B, 2009, 79, .	3.2	25
58	Superhard diamondlike<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BC</mml:mtext></mml:mrow><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math>: A first-principles investigation. Physical Review B, 2009, 80, .	3.2	24
59	Modelling zirconium hydrides using the special quasirandom structure approach. Physical Chemistry Chemical Physics, 2013, 15, 7599.	2.8	24
60	Order-to-disorder phase transformation in ion irradiated uranium-bearing delta-phase oxides RE6U1O12 (RE=Y, Gd, Ho, Yb, and Lu). Journal of Solid State Chemistry, 2010, 183, 844-848.	2.9	23
61	A computational method to identify interstitial sites in complex materials. Scripta Materialia, 2008, 58, 739-742.	5.2	22
62	Structures and stabilities of small carbon interstitial clusters in cubic silicon carbide. Acta Materialia, 2014, 62, 162-172.	7.9	22
63	A combined first-principles/CALPHAD modeling of the Alâ€“Ir system. Acta Materialia, 2006, 54, 4101-4110.	7.9	21
64	Computational investigation of constitutional liquation in Alâ€“Cu alloys. Acta Materialia, 2003, 51, 4447-4459.	7.9	20
65	Surface segregation of Pt in Î³â€²-Ni3Al: A first-principles study. Acta Materialia, 2007, 55, 1641-1647.	7.9	20
66	First principles prediction of vanadium and niobium nitrides with M2N3 stoichiometry. Scripta Materialia, 2010, 63, 532-535.	5.2	20
67	Using â€œradioparagenesisâ€• to design robust nuclear waste forms. Energy and Environmental Science, 2010, 3, 130-135.	30.8	20
68	Cation disorder in MgX2O4(X= Al, Ga, In) spinels from first principles. Physical Review B, 2012, 86, .	3.2	20
69	Accelerated atomistic simulation study on the stability and mobility of carbon tri-interstitial cluster in cubic SiC. Computational Materials Science, 2014, 89, 182-188.	3.0	20
70	Applications of Special Quasi-random Structures to High-Entropy Alloys. , 2016, , 333-368.		20
71	Native defects in LiNH<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: A first-principles study. Physical Review B, 2011, 84, .	3.2	19
72	Effects of Cr on the elastic properties of B2 NiAl: A first-principles study. Scripta Materialia, 2006, 55, 759-762.	5.2	18

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73	Microstructural Evolution of Secondary Phases in the Cast Duplex Stainless Steels CD3MN and CD3MWCuN. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2007, 38, 203-211.	2.2	18
74	The effect of Ti atom on hydrogenation of Al(111) surface: First-principles studies. International Journal of Hydrogen Energy, 2010, 35, 609-613.	7.1	18
75	Radioparagenesis: The formation of novel compounds and crystalline structures via radioactive decay. Philosophical Magazine Letters, 2010, 90, 435-446.	1.2	17
76	Special quasirandom structures for gadolinia-doped ceria and related materials. Physical Chemistry Chemical Physics, 2012, 14, 11737.	2.8	17
77	Gradient Array of Freely Suspended Nanomembranes. Advanced Functional Materials, 2006, 16, 27-32.	14.9	16
78	First-principles thermal equation of state of tungsten carbide. Computational Materials Science, 2012, 59, 41-47.	3.0	16
79	Special quasirandom structures for binary/ternary group IV random alloys. Chemical Physics Letters, 2010, 493, 97-102.	2.6	15
80	Ab initiomodeling of MAX phase solid solutions using the special quasirandom structure approach. Physical Chemistry Chemical Physics, 2018, 20, 1173-1180.	2.8	15
81	Segregation of Pt at clean surfaces of (Pt, Ni)3Al. Surface Science, 2007, 601, 376-380.	1.9	14
82	Implications of transmutation on the defect chemistry in crystalline waste forms. Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3261-3264.	1.4	14
83	Thermodynamic and mechanical stabilities of Î³â€²-Ir3(Al,W). Journal of Applied Physics, 2011, 109, 023504.	2.5	14
84	First-principles prediction of the thermodynamic stability of xenon in monoclinic, tetragonal, and yttrium-stabilized cubic ZrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review B, 2011, 83, .	3.2	14
85	A combined first-principles calculation and thermodynamic modeling of the Fâ€“Kâ€“Na system. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2006, 418, 161-171.	5.6	13
86	Noble gas bubbles in bcc metals: Ab initio-based theory and kinetic Monte Carlo modeling. Acta Materialia, 2021, 213, 116961.	7.9	13
87	Thermodynamic modeling of the indium-palladium system. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2002, 33, 3597-3603.	2.2	12
88	Pressureâ€“composition phase diagram of Tiâ€“<scp>C</scp> from first principles. Physica Status Solidi (B): Basic Research, 2014, 251, 533-536.	1.5	11
89	Systematic analysis on the primary radiation damage in Th1â^'xUxO2 fluorite systems. Journal of Nuclear Materials, 2020, 536, 152144.	2.7	11
90	Unveiling the atomic-scale origins of high damage tolerance of single-crystal high entropy alloys. Physical Review Materials, 2020, 4, .	2.4	11

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91	First-principles study of constitutional and thermal point defects in B2 PdIn. Intermetallics, 2006, 14, 248-254.	3.9	10
92	Charge compensation in an irradiation-induced phase of Î´-Sc4Zr3O12. Journal of Materials Science, 2009, 44, 4754-4757.	3.7	9
93	Ab initio theory of noble gas atoms in bcc transition metals. Physical Chemistry Chemical Physics, 2018, 20, 17048-17058.	2.8	9
94	Thermodynamic Assessment of the Mn-B System. Journal of Phase Equilibria and Diffusion, 2010, 31, 357-364.	1.4	7
95	Ab initio investigation and thermodynamic modeling of the Moâ€“Tiâ€“Zr system. Materialia, 2020, 10, 100701.	2.7	7
96	Symmetry breaking during defect self-organization under irradiation. Materials Theory, 2020, 4, .	4.3	7
97	Vacancy ordering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Co</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>Sn2: A first-principles study. Physical Review B, 2008, 78, .	3.2	6
98	Prediction of Irradiation Spectrum Effects in Pyrochlores. Jom, 2014, 66, 2578-2582.	1.9	6
99	Thermal stability of helium bubble superlattice in Mo under TEM in-situ heating. Journal of Nuclear Materials, 2018, 505, 207-211.	2.7	6
100	Bifurcation and Pattern Symmetry Selection in Reaction-Diffusion Systems with Kinetic Anisotropy. Scientific Reports, 2019, 9, 7835.	3.3	6
101	Understanding of fission products transport in SiC layer of TRISO fuels by nanoscale characterization and modeling. Journal of Nuclear Materials, 2019, 527, 151793.	2.7	6
102	Self-assembly of solid nanoclusters in molybdenum under gas ion implantation. Scripta Materialia, 2021, 194, 113651.	5.2	5
103	Unraveling small-scale defects in irradiated ThO2 using kinetic Monte Carlo simulations. Scripta Materialia, 2022, 214, 114684.	5.2	4
104	High-Resolution Scanning Transmission Electron Microscopy Study of Black Spot Defects in Ion Irradiated Silicon Carbide. Microscopy and Microanalysis, 2014, 20, 1824-1825.	0.4	3
105	Ab initio study and thermodynamic modeling of the Pd-Si-C system. Computational Materials Science, 2020, 171, 109238.	3.0	3
106	Revisiting the Phase Stability in Ni-X (X=Mo, Ti, In) Systems Using Ab Initio Calculations. Journal of Phase Equilibria and Diffusion, 2018, 39, 584-591.	1.4	2
107	Development of Fe-9Cr Alloy via High-Energy Ball Milling and Spark Plasma Sintering. Jom, 2019, 71, 2846-2855.	1.9	2
108	Influence of Alloying Elements and Effect of Stress on Anisotropic Hydrogen Diffusion in Zr-Based Alloys Predicted by Accelerated Kinetic Monte Carlo Simulations. Minerals, Metals and Materials Series, 2019, , 1815-1826.	0.4	2

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109	Bulk and surface diffusion of neodymium in alpha-uranium: Ab initio calculations and kinetic Monte Carlo simulations. Journal of Nuclear Materials, 2021, 557, 153307.	2.7	1
110	B2 Phases and their Defect Structures: Part I. Ab Initio Enthalpy of Formation and Enthalpy of Mixing in the Al-Ni-Pt-Ru System. Materials Research Society Symposia Proceedings, 2004, 842, 239.	0.1	0
111	Inside Front Cover: Freely Suspended Layer-by-Layer Nanomembranes: Testing Micromechanical Properties (Adv. Funct. Mater. 5/2005). Advanced Functional Materials, 2005, 15, NA-NA.	14.9	0
112	Inside Front Cover: Trilayered Ceramicâ€“Metalâ€“Polymer Microcantilevers with Dramatically Enhanced Thermal Sensitivity (Adv. Mater. 9/2006). Advanced Materials, 2006, 18, NA-NA.	21.0	0
113	Influence of Alloying Elements and Effect of Stress on Anisotropic Hydrogen Diffusion in Zr-Based Alloys Predicted by Accelerated Kinetic Monte Carlo Simulations. Minerals, Metals and Materials Series, 2018, , 599-610.	0.4	0