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	Unraveling small-scale defects in irradiated ThO2 using kinetic Monte Carlo simulations. Scripta Materialia, 2022, 214, 114684.	5.2	4
2	Self-assembly of solid nanoclusters in molybdenum under gas ion implantation. Scripta Materialia, 2021, 194, 113651.	5.2	5
3	Noble gas bubbles in bcc metals: Ab initio-based theory and kinetic Monte Carlo modeling. Acta Materialia, 2021, 213, 116961.	7.9	13
4	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
5	Ab initio study and thermodynamic modeling of the Pd-Si-C system. Computational Materials Science, 2020, 171, 109238.	3.0	3
6	Ab initio investigation and thermodynamic modeling of the Moâ€“Tiâ€“Zr system. Materialia, 2020, 10, 100701.	2.7	7
7	Systematic analysis on the primary radiation damage in Th1â^'xUxO2 fluorite systems. Journal of Nuclear Materials, 2020, 536, 152144.	2.7	11
8	Unveiling the atomic-scale origins of high damage tolerance of single-crystal high entropy alloys. Physical Review Materials, 2020, 4, .	2.4	11
9	Symmetry breaking during defect self-organization under irradiation. Materials Theory, 2020, 4, .	4.3	7
10	Bifurcation and Pattern Symmetry Selection in Reaction-Diffusion Systems with Kinetic Anisotropy. Scientific Reports, 2019, 9, 7835.	3.3	6
11	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
12	Development of Fe-9Cr Alloy via High-Energy Ball Milling and Spark Plasma Sintering. Jom, 2019, 71, 2846-2855.	1.9	2
13	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
14	Theoretical prediction and atomic kinetic Monte Carlo simulations of void superlattice self-organization under irradiation. Scientific Reports, 2018, 8, 6629.	3.3	27
15	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
16	Ab initiomodeling of MAX phase solid solutions using the special quasirandom structure approach. Physical Chemistry Chemical Physics, 2018, 20, 1173-1180.	2.8	15
17	Thermal stability of helium bubble superlattice in Mo under TEM in-situ heating. Journal of Nuclear Materials, 2018, 505, 207-211.	2.7	6
18	Formation and self-organization of void superlattices under irradiation: A phase field study. Materialia, 2018, 1, 78-88.	2.7	39

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19	Ab initio theory of noble gas atoms in bcc transition metals. Physical Chemistry Chemical Physics, 2018, 20, 17048-17058.	2.8	9
20	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
21	Anisotropic hydrogen diffusion in Î±-Zr and Zircaloy predicted by accelerated kinetic Monte Carlo simulations. Scientific Reports, 2017, 7, 41033.	3.3	33
22	Using Machine Learning To Identify Factors That Govern Amorphization of Irradiated Pyrochlores. Chemistry of Materials, 2017, 29, 2574-2583.	6.7	33
23	Applications of Special Quasi-random Structures to High-Entropy Alloys. , 2016, , 333-368.		20
24	EfficientAbÂinitioModeling of Random Multicomponent Alloys. Physical Review Letters, 2016, 116, 105501.	7.8	93
25	Band-Gap and Band-Edge Engineering of Multicomponent Garnet Scintillators from First Principles. Physical Review Applied, 2015, 4, .	3.8	62
26	Opposite correlations between cation disordering and amorphization resistance in spinels versus pyrochlores. Nature Communications, 2015, 6, 8750.	12.8	62
27	Prediction of Irradiation Spectrum Effects in Pyrochlores. Jom, 2014, 66, 2578-2582.	1.9	6
28	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
29	Effect of Grain Boundary Stresses on Sink Strength. Materials Research Letters, 2014, 2, 100-106.	8.7	51
30	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
31	Structures and stabilities of small carbon interstitial clusters in cubic silicon carbide. Acta Materialia, 2014, 62, 162-172.	7.9	22
32	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
33	Nuclear wasteform materials: Atomistic simulation case studies. Journal of Nuclear Materials, 2013, 441, 29-39.	2.7	45
34	Amorphization Driven by Defect-Induced Mechanical Instability. Physical Review Letters, 2013, 111, 155501.	7.8	35
35	Modelling zirconium hydrides using the special quasirandom structure approach. Physical Chemistry Chemical Physics, 2013, 15, 7599.	2.8	24
36	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

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37	Unexpected strain-stiffening in crystalline solids. Nature, 2013, 496, 339-342.	27.8	64
38	Role of Antisite Disorder on Preamorphization Swelling in Titanate Pyrochlores. Physical Review Letters, 2012, 108, 195504.	7.8	85
39	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
40	Special quasirandom structures for gadolinia-doped ceria and related materials. Physical Chemistry Chemical Physics, 2012, 14, 11737.	2.8	17
41	Effects of Cu content on the precipitation process of Alâ€“Znâ€“Mg alloys. Journal of Materials Science, 2012, 47, 8174-8187.	3.7	34
42	Cation disorder in MgX2O4(X= Al, Ga, In) spinels from first principles. Physical Review B, 2012, 86, .	3.2	20
43	First-principles thermal equation of state of tungsten carbide. Computational Materials Science, 2012, 59, 41-47.	3.0	16
44	First-principles based modeling of hydrogen permeation through Pdâ€“Cu alloys. International Journal of Hydrogen Energy, 2012, 37, 12760-12764.	7.1	28
45	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
46	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:mml:	3.2	288
47	Thermodynamic and mechanical stabilities of Î³â€²-Ir3(Al,W). Journal of Applied Physics, 2011, 109, 023504.	2.5	14
48	Phase stability 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: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
49	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
50	Native defects in LiNH<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>: A first-principles study. Physical Review B, 2011, 84, .	3.2	19
51	Thermodynamic Assessment of the Mn-B System. Journal of Phase Equilibria and Diffusion, 2010, 31, 357-364.	1.4	7
52	First principles prediction of vanadium and niobium nitrides with M2N3 stoichiometry. Scripta Materialia, 2010, 63, 532-535.	5.2	20
53	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
54	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

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55	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
56	Special quasirandom structures for binary/ternary group IV random alloys. Chemical Physics Letters, 2010, 493, 97-102.	2.6	15
57	Radioparagenesis: The formation of novel compounds and crystalline structures via radioactive decay. Philosophical Magazine Letters, 2010, 90, 435-446.	1.2	17
58	Deviations from Vegardâ€™s law in ternary III-V alloys. Physical Review B, 2010, 82, .	3.2	89
59	Using â€œradioparagenesisâ€• to design robust nuclear waste forms. Energy and Environmental Science, 2010, 3, 130-135.	30.8	20
60	First-principles prediction of disordering tendencies in pyrochlore oxides. Physical Review B, 2009, 79, .	3.2	140
61	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> 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
62	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
63	First-principles prediction of mechanical properties of gamma-boron. Applied Physics Letters, 2009, 94, 191906.	3.3	40
64	First-principles study of ternary bcc alloys using special quasi-random structures. Acta Materialia, 2009, 57, 4716-4726.	7.9	66
65	Charge compensation in an irradiation-induced phase of Î´-Sc4Zr3O12. Journal of Materials Science, 2009, 44, 4754-4757.	3.7	9
66	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
67	E centers in ternary Si1âˆ’xâˆ’yGexSny random alloys. Applied Physics Letters, 2009, 95, .	3.3	64
68	Defect interactions in Sn1âˆ’xGex random alloys. Applied Physics Letters, 2009, 94, 252104.	3.3	65
69	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:mi>:m A first-principles investigation. Physical Review B, 2009, 80, .	3.2	24
70	Thermodynamic and Mechanical Stabilities of Tantalum Nitride. Physical Review Letters, 2009, 103, 185501.	7.8	68
71	Point defect thermodynamics and diffusion in Fe3C: A first-principles study. Acta Materialia, 2008, 56, 3236-3244.	7.9	26
72	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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73	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
74	A computational method to identify interstitial sites in complex materials. Scripta Materialia, 2008, 58, 739-742.	5.2	22
75	First-principles study of Co3(Al,W) alloys using special quasi-random structures. Scripta Materialia, 2008, 59, 1075-1078.	5.2	85
76	Structural, elastic, and electronic properties of Fe3C from first principles. Journal of Applied Physics, 2008, 103, .	2.5	134
77	First-principles study of structural, elastic, and electronic properties of chromium carbides. Applied Physics Letters, 2008, 92, .	3.3	116
78	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></mml:mrow></mml:msub></mml:mrow></mml:math> Electronic structure calculations. Physical Review B, 2008, 78, .	3.2	63
79	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:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> A first-principles study. Physical Review B, 2008, 78, .	3.2	6
80	Segregation of Pt at clean surfaces of (Pt, Ni)3Al. Surface Science, 2007, 601, 376-380.	1.9	14
81	Site preference of early transition metal elements in C15 NbCr2. Acta Materialia, 2007, 55, 1599-1605.	7.9	47
82	Surface segregation of Pt in Î³â€²-Ni3Al: A first-principles study. Acta Materialia, 2007, 55, 1641-1647.	7.9	20
83	Site preference of transition-metal elements in B2 NiAl: A comprehensive study. Acta Materialia, 2007, 55, 4799-4806.	7.9	78
84	Pressure-Induced Cubic to Monoclinic Phase Transformation in Erbium Sesquioxide Er2O3. Inorganic Chemistry, 2007, 46, 6164-6169.	4.0	71
85	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
86	First-principles study of constitutional and thermal point defects in B2 PdIn. Intermetallics, 2006, 14, 248-254.	3.9	10
87	Site preference of ternary alloying elements in Ni3Al: A first-principles study. Acta Materialia, 2006, 54, 1147-1154.	7.9	130
88	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
89	A combined first-principles/CALPHAD modeling of the Alâ€“Ir system. Acta Materialia, 2006, 54, 4101-4110.	7.9	21
90	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

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91	A first-principles study of the site preference of Cr in B2 NiAl. Scripta Materialia, 2006, 54, 405-410.	5.2	25
92	Site preference of transition metal elements in Ni3Al. Scripta Materialia, 2006, 55, 433-436.	5.2	133
93	Effects of Cr on the elastic properties of B2 NiAl: A first-principles study. Scripta Materialia, 2006, 55, 759-762.	5.2	18
94	Gradient Array of Freely Suspended Nanomembranes. Advanced Functional Materials, 2006, 16, 27-32.	14.9	16
95	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
96	Trilayered Ceramicâ€“Metalâ€“Polymer Microcantilevers with Dramatically Enhanced Thermal Sensitivity. Advanced Materials, 2006, 18, 1157-1161.	21.0	29
97	Freestanding Nanostructures via Layer-by-Layer Assembly. Advanced Materials, 2006, 18, 829-840.	21.0	387
98	Freestanding 2D Arrays of Silver Nanorods. Advanced Materials, 2006, 18, 2895-2899.	21.0	32
99	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
100	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
101	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
102	First-principles study of constitutional point defects in B2 NiAl using special quasirandom structures. Acta Materialia, 2005, 53, 2643-2652.	7.9	42
103	Freely Suspended Layer-by-Layer Nanomembranes: Testing Micromechanical Properties. Advanced Functional Materials, 2005, 15, 771-780.	14.9	182
104	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
105	Freely Suspended Gold Nanoparticle Arrays. Advanced Materials, 2005, 17, 1669-1673.	21.0	74
106	Strain-Sensitive Raman Modes of Carbon Nanotubes in Deflecting Freely Suspended Nanomembranes. Advanced Materials, 2005, 17, 2127-2131.	21.0	61
107	First-principles study of phase stability in pseudobinary(Ni1â^'xPtx)3Alalloys. Physical Review B, 2005, 72, .	3.2	38
108	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

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109	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
110	First-principles study of binary bcc alloys using special quasirandom structures. Physical Review B, 2004, 69, .	3.2	266
111	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
112	Computational investigation of constitutional liquation in Alâ€“Cu alloys. Acta Materialia, 2003, 51, 4447-4459.	7.9	20
113	Thermodynamic modeling of the indium-palladium system. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2002, 33, 3597-3603.	2.2	12