Fei Gao

List of Publications by Year
in descending order

373 papers	13,593 citations	25034 57 h-index	34986 98 g-index

375 all docs	375 docs citations	375 times ranked	11255 citing authors

#	Article	IF	Citations
1	Lewis Acidâ€“Base Interactions between Polysulfides and Metal Organic Framework in Lithium Sulfur Batteries. Nano Letters, 2014, 14, 2345-2352.	9.1	623
2	Enhancing radiation tolerance by controlling defect mobility and migration pathways in multicomponent single-phase alloys. Nature Communications, 2016, 7, 13564.	12.8	533
3	The primary damage state in fcc, bcc and hcp metals as seen in molecular dynamics simulations. Journal of Nuclear Materials, 2000, 276, 1-12.	2.7	326
4	Tensile Strain Switched Ferromagnetism in Layered NbS₂ and NbSe₂. ACS Nano, 2012, 6, 9727-9736.	14.6	325
5	Probing grain boundary sink strength at the nanoscale: Energetics and length scales of vacancy and interstitial absorption by grain boundaries in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Fe. Physical Review B, 2012, 85, .	3.2	285
6	Evolution of Lattice Structure and Chemical Composition of the Surface Reconstruction Layer in Li_{1.2}Ni_{0.2}Mn_{0.6}O₂ Cathode Material for Lithium Ion Batteries. Nano Letters, 2015, 15, 514-522.	9.1	261
7	In Situ TEM Investigation of Congruent Phase Transition and Structural Evolution of Nanostructured Silicon/Carbon Anode for Lithium Ion Batteries. Nano Letters, 2012, 12, 1624-1632.	9.1	256
8	Conflicting Roles of Nickel in Controlling Cathode Performance in Lithium Ion Batteries. Nano Letters, 2012, 12, 5186-5191.	9.1	231
9	Radiation-induced segregation on defect clusters in single-phase concentrated solid-solution alloys. Acta Materialia, 2017, 127, 98-107.	7.9	212
10	Atomic scale simulation of defect production in irradiated 3C-SiC. Journal of Applied Physics, 2001, 90, 2303-2309.	2.5	211
11	Computer simulation of defect production by displacement cascades in metals. Nuclear Instruments & Methods in Physics Research B, 1995, 102, 37-46.	1.4	178
12	A germanium hole spin qubit. Nature Communications, 2018, 9, 3902.	12.8	170
13	Analytic modified embedded atom potentials for HCP metals. Journal of Physics Condensed Matter, 2001, 13, 1193-1213.	1.8	157
14	Signal variance in gamma-ray detectorsâ€”A review. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2006, 565, 637-649.	1.6	148
15	Point-defect and threshold displacement energies in Ni₃Al I. Point-defect properties. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1993, 67, 275-288.	0.6	143
16	Cascade overlap and amorphization in3Câ^'SiC:Defect accumulation, topological features, and disordering. Physical Review B, 2002, 66, .	3.2	135
17	Electronic Origin for the Phase Transition from Amorphous Li_xSi to Crystalline Li₁₅Si₄. ACS Nano, 2013, 7, 6303-6309.	14.6	135
18	Properties of helium defects in bcc and fcc metals investigated with density functional theory. Physical Review B, 2009, 80, .	3.2	134

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19	Probing the Degradation Mechanism of Li₂MnO₃ Cathode for Li-Ion Batteries. Chemistry of Materials, 2015, 27, 975-982.	6.7	130
20	A molecular dynamics study of temperature effects on defect production by displacement cascades in Î±-iron. Journal of Nuclear Materials, 1997, 249, 77-86.	2.7	129
21	Reaction heterogeneity in practical high-energy lithiumâ€“sulfur pouch cells. Energy and Environmental Science, 2020, 13, 3620-3632.	30.8	127
22	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. Acta Materialia, 2020, 196, 133-143.	7.9	124
23	Defect production due to displacement cascades in metals as revealed by computer simulation. Journal of Nuclear Materials, 1997, 251, 1-12.	2.7	116
24	Atomistic study of intrinsic defect migration in 3C-SiC. Physical Review B, 2004, 69, .	3.2	115
25	Grain growth and phase stability of nanocrystalline cubic zirconia under ion irradiation. Physical Review B, 2010, 82, .	3.2	115
26	In situnitrogen-doped graphene grown from polydimethylsiloxane by plasma enhanced chemical vapor deposition. Nanoscale, 2013, 5, 600-605.	5.6	114
27	Atomic-scale simulation of 50 keV Si displacement cascades in Î²-SiC. Physical Review B, 2000, 63, .	3.2	113
28	Shockwave generates < 100 > dislocation loops in bcc iron. Nature Communications, 2018, 9, 4880.	12.8	106
29	Defect production, multiple ionâ€“solid interactions and amorphization in SiC. Nuclear Instruments & Methods in Physics Research B, 2002, 191, 487-496.	1.4	104
30	Electronic structures and magnetic properties of MoS2 nanostructures: atomic defects, nanoholes, nanodots and antidots. Physical Chemistry Chemical Physics, 2013, 15, 10385.	2.8	104
31	Modified analytical interatomic potential for a Wâ€“H system with defects. Journal of Nuclear Materials, 2011, 408, 12-17.	2.7	98
32	Adsorption of hydrogen on boron-doped graphene: A first-principles prediction. Journal of Applied Physics, 2009, 105, .	2.5	96
33	Ab initioand empirical-potential studies of defect properties in3Câ^'SiC. Physical Review B, 2001, 64, .	3.2	95
34	Recovery of close Frenkel pairs produced by low energy recoils in SiC. Journal of Applied Physics, 2003, 94, 4348-4356.	2.5	95
35	A molecular dynamics study of high-energy displacement cascades in Î±-zirconium. Journal of Nuclear Materials, 1998, 254, 191-204.	2.7	92
36	Diffusion of He interstitials in grain boundaries in Î±-Fe. Journal of Nuclear Materials, 2006, 351, 133-140.	2.7	90

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37	Dopant Segregation Boosting Highâ€Voltage Cyclability of Layered Cathode for Sodium Ion Batteries. Advanced Materials, 2019, 31, e1904816.	21.0	89
38	Temperature-dependence of defect creation and clustering by displacement cascades in Î±-zirconium. Journal of Nuclear Materials, 2001, 294, 288-298.	2.7	88
39	Atomistic Conversion Reaction Mechanism of WO₃ in Secondary Ion Batteries of Li, Na, and Ca. Angewandte Chemie - International Edition, 2016, 55, 6244-6247.	13.8	86
40	A new Feâ€“He interatomic potential based on ab initio calculations in Î±-Fe. Journal of Nuclear Materials, 2011, 418, 115-120.	2.7	83
41	Empirical potential approach for defect properties in 3C-SiC. Nuclear Instruments & Methods in Physics Research B, 2002, 191, 504-508.	1.4	81
42	Threshold displacement energy in GaN: Ab initio molecular dynamics study. Journal of Applied Physics, 2009, 105, .	2.5	79
43	Analytical Wâ€“He and Hâ€“He interatomic potentials for a Wâ€“Hâ€“He system. Journal of Nuclear Materials, 2012, 426, 31-37.	2.7	76
44	Evidencing the existence of exciting half-metallicity in two-dimensional TiCl3 and VCl3 sheets. Scientific Reports, 2016, 6, 19407.	3.3	76
45	Formation of stacking-fault tetrahedra in collision cascades. Applied Physics Letters, 1999, 74, 2720-2722.	3.3	74
46	Defect-Enhanced Charge Transfer by Ion-Solid Interactions in SiC using Large-ScaleAbÂInitioMolecular Dynamics Simulations. Physical Review Letters, 2009, 103, 027405.	7.8	74
47	Interaction of helium atoms with edge dislocations in Î±-Fe. Journal of Nuclear Materials, 2006, 351, 141-148.	2.7	71
48	Molecular dynamics study of displacement cascades in Ni₃Al I. General features and defect production efficiency. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1995, 71, 43-64.	0.6	70
49	Energetic driving force for preferential binding of self-interstitial atoms to Fe grain boundaries over vacancies. Scripta Materialia, 2011, 64, 908-911.	5.2	69
50	Atomistic simulations of the mechanical properties of silicon carbide nanowires. Physical Review B, 2008, 77, .	3.2	67
51	Properties and evolution of sessile interstitial clusters produced by displacement cascades in Î±-iron. Journal of Nuclear Materials, 2000, 276, 213-220.	2.7	65
52	Computer simulation of disordering and amorphization by Si and Au recoils in 3Câ€“SiC. Journal of Applied Physics, 2001, 89, 4275-4281.	2.5	65
53	Phase-field modeling of void migration and growth kinetics in materials under irradiation and temperature field. Journal of Nuclear Materials, 2010, 407, 119-125.	2.7	63
54	Modification of Defect Structures in Graphene by Electron Irradiation: Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2012, 116, 16070-16079.	3.1	61

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55	Adsorption-induced magnetic properties and metallic behavior of graphene. Applied Physics Letters, 2009, 95, 123119.	3.3	60
56	Electronic and magnetic properties of metal-doped BN sheet: A first-principles study. Physical Chemistry Chemical Physics, 2010, 12, 7588.	2.8	59
57	Molecular dynamics simulation of helium cluster diffusion and bubble formation in bulk tungsten. Journal of Nuclear Materials, 2014, 455, 544-548.	2.7	58
58	Ultrafast coherent control of a hole spin qubit in a germanium quantum dot. Nature Communications, 2022, 13, 206.	12.8	58
59	New interatomic potentials of W, Re and W-Re alloy for radiation defects. Journal of Nuclear Materials, 2018, 502, 141-153.	2.7	57
60	The effects of electron-phonon coupling on defect production by displacement cascades in -iron. Modelling and Simulation in Materials Science and Engineering, 1998, 6, 543-556.	2.0	56
61	Effects of local structure on helium bubble growth in bulk and at grain boundaries of bcc iron: A molecular dynamics study. Acta Materialia, 2015, 97, 86-93.	7.9	54
62	Point-defect and threshold displacement energies in Ni₃Al II. Events at the displacement threshold. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1993, 67, 289-306.	0.6	52
63	Electron-Rich Driven Electrochemical Solid-State Amorphization in Liâ€“Si Alloys. Nano Letters, 2013, 13, 4511-4516.	9.1	51
64	Threshold displacement energies and defect formation energies in Y₂Ti₂O₇. Journal of Physics Condensed Matter, 2010, 22, 415801.	1.8	50
65	Phase-field simulations of intragranular fission gas bubble evolution in UO2 under post-irradiation thermal annealing. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 62-67.	1.4	50
66	Molecular-confinement of polysulfides within mesoscale electrodes for the practical application of lithium sulfur batteries. Nano Energy, 2015, 13, 267-274.	16.0	50
67	Ab initio investigation of phase stability of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>Y</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mrow> <mml:mtext xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>Y</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:mtext>Physical Review B, 2009, 80, .	3.2	48
68	Computer simulation of electron thermalization in CsI and CsI(Tl). Journal of Applied Physics, 2011, 110, .	2.5	47
69	Controlling Adsorption Structure of Eosin Y Dye on Nanocrystalline TiO₂ Films for Improved Photovoltaic Performances. Journal of Physical Chemistry C, 2013, 117, 14659-14666.	3.1	47
70	Atomic-scale simulation of displacement cascades and amorphization in Î²-SiC. Nuclear Instruments & Methods in Physics Research B, 2001, 180, 176-186.	1.4	46
71	Enhanced void swelling in NiCoFeCrPd high-entropy alloy by indentation-induced dislocations. Materials Research Letters, 2018, 6, 584-591.	8.7	46
72	Atomistic simulations of the size, orientation, and temperature dependence of tensile behavior in GaN nanowires. Physical Review B, 2007, 76, .	3.2	45

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73	Electronic and magnetic properties of substituted BN sheets: A density functional theory study. Physical Chemistry Chemical Physics, 2011, 13, 7378.	2.8	45
74	Atomistic studies of nucleation of He clusters and bubbles in bcc iron. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 68-71.	1.4	45
75	Atomistic simulation of helium-defect interaction in alpha-iron. Applied Physics Letters, 2006, 88, 091915.	3.3	44
76	Structural and bonding properties of stannate pyrochlores: A density functional theory investigation. Computational Materials Science, 2008, 42, 653-658.	3.0	44
77	First principles prediction of nitrogen-doped carbon nanotubes as a high-performance cathode for Liâ€“S batteries. RSC Advances, 2013, 3, 16775.	3.6	44
78	Native defect properties in Î²-SiC: Ab initio and empirical potential calculations. Nuclear Instruments & Methods in Physics Research B, 2001, 180, 286-292.	1.4	43
79	Atomistic simulation of the size and orientation dependences of thermal conductivity in GaN nanowires. Applied Physics Letters, 2007, 90, 161923.	3.3	43
80	Computer simulation of the light yield nonlinearity of inorganic scintillators. Journal of Applied Physics, 2009, 105, .	2.5	43
81	Zirconate pyrochlores under high pressure. Physical Chemistry Chemical Physics, 2010, 12, 12472.	2.8	43
82	Computer simulation of displacement cascade effects in metals. Radiation Effects and Defects in Solids, 1997, 141, 283-310.	1.2	42
83	Atomistic study of the migration of di- and tri-interstitials in silicon. Physical Review B, 2005, 71, .	3.2	42
84	First-principles study of electronic properties of La2Hf2O7 and Gd2Hf2O7. Journal of Applied Physics, 2007, 102, 063704.	2.5	42
85	Energy dissipation and defect generation in nanocrystalline silicon carbide. Physical Review B, 2010, 81, .	3.2	42
86	Mechanical properties and elastic constants due to damage accumulation and amorphization in SiC. Physical Review B, 2004, 69, .	3.2	41
87	Intrinsic defect properties in GaN calculated byab initioand empirical potential methods. Physical Review B, 2004, 70, .	3.2	41
88	Monte Carlo simulations of defect recovery within a 10 keV collision cascade in 3Câ€“SiC. Journal of Applied Physics, 2007, 102, .	2.5	41
89	Electronic and optical properties of two-dimensional covalent organic frameworks. Journal of Materials Chemistry, 2012, 22, 16964.	6.7	41
90	Diffusion of small He clusters in bulk and grain boundaries in Î±-Fe. Journal of Nuclear Materials, 2013, 442, S667-S673.	2.7	41

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91	Atomistic modeling of helium interacting with screw dislocations in Î±-Fe. Journal of Nuclear Materials, 2007, 367-370, 311-315.	2.7	40
92	Tensile and compressive mechanical behavior of twinned silicon carbide nanowires. Acta Materialia, 2010, 58, 1963-1971.	7.9	40
93	Siteâ€Controlled Uniform Ge/Si Hut Wires with Electrically Tunable Spinâ€“Orbit Coupling. Advanced Materials, 2020, 32, e1906523.	21.0	40
94	Migration of vacancies, He interstitials and He-vacancy clusters at grain boundaries in Î±-Fe. Journal of Nuclear Materials, 2009, 386-388, 390-394.	2.7	39
95	First-principles calculations of pressure-induced phase transformation in AlN and GaN. Computational Materials Science, 2010, 48, 768-772.	3.0	39
96	Diffusion of He interstitial and di-He cluster at grain boundaries in Î±-Fe. Journal of Nuclear Materials, 2007, 367-370, 446-450.	2.7	38
97	First principles study of electronic properties of gallium nitride nanowires grown along different crystal directions. Computational Materials Science, 2010, 50, 344-348.	3.0	38
98	Novel Electronic and Magnetic Properties of Graphene Nanoflakes in a Boron Nitride Layer. Journal of Physical Chemistry C, 2012, 116, 7581-7586.	3.1	38
99	Molecular dynamics simulations of irradiation cascades in alpha-zirconium under macroscopic strain. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 95-99.	1.4	38
100	Perspectives on multiscale modelling and experiments to accelerate materials development for fusion. Journal of Nuclear Materials, 2021, 554, 153113.	2.7	37
101	Amorphization of silicon carbide by carbon displacement. Applied Physics Letters, 2004, 84, 3909-3911.	3.3	36
102	Interplay between atomic disorder, lattice swelling, and defect energy in ion-irradiation-induced amorphization of SiC. Physical Review B, 2014, 90, .	3.2	36
103	Atomistic simulations of helium clustering and grain boundary reconstruction in alpha-iron. Acta Materialia, 2015, 82, 275-286.	7.9	36
104	Coupling a Germanium Hut Wire Hole Quantum Dot to a Superconducting Microwave Resonator. Nano Letters, 2018, 18, 2091-2097.	9.1	36
105	Molecular dynamics simulations of high-energy radiation damage in W and Wâ€“Re alloys. Journal of Nuclear Materials, 2019, 524, 9-20.	2.7	36
106	The influence of strain on defect generation by displacement cascades in Î±-iron. Nuclear Instruments & Methods in Physics Research B, 2001, 180, 187-193.	1.4	35
107	The effects of interfaces on radiation damage production in layered metal composites. Journal of Nuclear Materials, 2004, 329-333, 924-928.	2.7	35
108	First-principles calculation of structural and energetic properties for A₂Ti₂O₇ (A = Lu, Er, Y, Gd, Sm, Nd, La). Journal of Materials Research, 2009, 24, 1335-1341.	2.6	35

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109	Molecular dynamics modeling of the thermal conductivity of irradiated SiC as a function of cascade overlap. Journal of Applied Physics, 2007, 101, 023527.	2.5	34
110	Understanding the presence of vacancy clusters in ZnO from a kinetic perspective. Applied Physics Letters, 2014, 104, 252101.	3.3	34
111	Enhanced Radiation-tolerant Oxide Dispersion Strengthened Steel and its Microstructure Evolution under Helium-implantation and Heavy-ion Irradiation. Scientific Reports, 2017, 7, 40343.	3.3	34
112	Interstitial migration behavior and defect evolution in ion irradiated pure nickel and Ni-xFe binary alloys. Journal of Nuclear Materials, 2018, 509, 237-244.	2.7	34
113	Study of loopâ€“loop and loopâ€“edge dislocation interactions in bcc iron. Journal of Nuclear Materials, 2000, 283-287, 784-788.	2.7	33
114	Damage accumulation and defect relaxation in4Hâ^'SiC. Physical Review B, 2004, 70, .	3.2	33
115	Monte Carlo method for simulating Î³-ray interaction with materials: A case study on Si. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2007, 579, 292-296.	1.6	33
116	Ab initio study of formation, migration and binding properties of heliumâ€“vacancy clusters in aluminum. Physica B: Condensed Matter, 2008, 403, 2719-2724.	2.7	32
117	Monte Carlo simulations of electron thermalization in alkali iodide and alkaline-earth fluoride scintillators. Journal of Applied Physics, 2012, 112, .	2.5	32
118	Regulating energy transfer of excited carriers and the case for excitation-induced hydrogen dissociation on hydrogenated graphene. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 908-911.	7.1	32
119	The interactions between rhenium and interstitial-type defects in bulk tungsten: A combined study by molecular dynamics and molecular statics simulations. Journal of Nuclear Materials, 2019, 522, 200-211.	2.7	32
120	Primary damage states produced by Si and Au recoils in SiC: A molecular dynamics and experimental investigation. Physical Review B, 2001, 63, .	3.2	31
121	Three-dimensional metal-intercalated covalent organic frameworks for near-ambient energy storage. Scientific Reports, 2013, 3, 1882.	3.3	31
122	Kinetic Monte Carlo simulations of excitation density dependent scintillation in Cs<scp>I</scp> and Cs<scp>I</scp>(<scp>T</scp>l). Physica Status Solidi (B): Basic Research, 2013, 250, 1532-1540.	1.5	31
123	Blunting of a brittle crack at grain boundaries: An atomistic study in BCC Iron. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 576, 231-238.	5.6	31
124	Binding energetics of substitutional and interstitial helium and di-helium defects with grain boundary structure in Î±-Fe. Journal of Applied Physics, 2014, 115, .	2.5	31
125	Energetics of vacancy segregation to [100] symmetric tilt grain boundaries in bcc tungsten. Scientific Reports, 2016, 6, 36955.	3.3	31
126	Kinetic Monte Carlo Annealing Simulation of Damage Produced by Cascades in Alpha-Iron. Materials Research Society Symposia Proceedings, 1998, 540, 703.	0.1	30

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127	Gamma-ray interaction in Ge: A Monte Carlo simulation. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 286-290.	1.4	30
128	Modeling of Heâ€“defect interactions in ferritic alloys for fusion. Journal of Nuclear Materials, 2008, 382, 134-142.	2.7	30
129	Dynamic interactions of helium-vacancy clusters with edge dislocations in Î±-Fe. Physica B: Condensed Matter, 2010, 405, 1754-1758.	2.7	30
130	Synthesis of Câ€“N dual-doped Cr₂O₃ visible light-driven photocatalysts derived from metalorganic framework (MOF) for cyclohexane oxidation. RSC Advances, 2016, 6, 84871-84881.	3.6	30
131	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. Journal of Alloys and Compounds, 2019, 775, 1184-1198.	5.5	30
132	Molecular dynamics study of displacement cascades in Ni3Al II. Kinetics, disordering and atomic mixing. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1995, 71, 65-84.	0.6	29
133	Atomic-level study of melting behavior of GaN nanotubes. Journal of Applied Physics, 2006, 100, 063503.	2.5	29
134	Defects in gallium nitride nanowires: First principles calculations. Journal of Applied Physics, 2010, 108, 044305.	2.5	29
135	Atomic-scale modeling of interactions of helium, vacancies and heliumâ€“vacancy clusters with screw dislocations in alpha-iron. Philosophical Magazine, 2010, 90, 885-895.	1.6	29
136	Computer simulations of interstitial loop growth kinetics in irradiated bcc Fe. Journal of Nuclear Materials, 2012, 427, 259-267.	2.7	29
137	Carrier-Multiplication-Induced Structural Change during Ultrafast Carrier Relaxation and Nonthermal Phase Transition in Semiconductors. Physical Review Letters, 2016, 117, 126402.	7.8	29
138	Spin and band-gap engineering in copper-doped BN sheet. Chemical Physics Letters, 2010, 491, 203-207.	2.6	28
139	A comparative study of the structure and energetics of elementary defects in 3C- and 4H-SiC. Journal of Physics Condensed Matter, 2004, 16, 1307-1323.	1.8	27
140	H+ diffusion and electrochemical stability of Li1+x+yAlxTi2â^'xSiyP3â^'yO12 glass in aqueous Li/air battery electrolytes. Journal of Power Sources, 2012, 214, 292-297.	7.8	27
141	Heâ€“V cluster nucleation and growth in Î±-Fe grain boundaries. Acta Materialia, 2017, 124, 544-555.	7.9	27
142	Self-healing mechanism of irradiation defects in nickelâ€“graphene nanocomposite: An energetic and kinetic perspective. Journal of Alloys and Compounds, 2018, 765, 253-263.	5.5	27
143	Interaction of heliumâ€“vacancy clusters with edge dislocations in Î±-Fe. Nuclear Instruments & Methods in Physics Research B, 2007, 265, 541-546.	1.4	26
144	Irradiation-induced defect clustering and amorphization in silicon carbide. Journal of Materials Research, 2010, 25, 2349-2353.	2.6	26

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145	Ab initio study of intrinsic, H, and He point defects in hcp-Er. Journal of Applied Physics, 2010, 107, 054903.	2.5	26
146	Dislocation-accelerated void formation under irradiation in zirconium. Acta Materialia, 2015, 82, 94-99.	7.9	26
147	Embedded-atom method potential for modeling hydrogen and hydrogen-defect interaction in tungsten. Journal of Physics Condensed Matter, 2017, 29, 435401.	1.8	26
148	A first-principles study of the structural, mechanical and electronic properties of precipitates of Al₂Cu in Alâ€“Cu alloys. Physical Chemistry Chemical Physics, 2018, 20, 967-976.	2.8	26
149	Development of the interatomic potentials for W-Ta system. Computational Materials Science, 2019, 163, 91-99.	3.0	26
150	Codoping of magnesium with oxygen in gallium nitride nanowires. Applied Physics Letters, 2010, 96, .	3.3	25
151	Molecular dynamics simulation of the structural, elastic, and thermal properties of pyrochlores. RSC Advances, 2016, 6, 41410-41419.	3.6	25
152	Irradiation effects of medium-entropy alloy NiCoCr with and without pre-indentation. Journal of Nuclear Materials, 2019, 524, 60-66.	2.7	25
153	Finding possible transition states of defects in silicon-carbide and alpha-iron using the dimer method. Nuclear Instruments & Methods in Physics Research B, 2003, 202, 1-7.	1.4	24
154	First-principles study of energetic and electronic properties of A2Ti2O7 (A=Sm, Gd, Er) pyrochlore. Journal of Applied Physics, 2008, 104, .	2.5	24
155	Molecular dynamics simulation of interaction of H with vacancy in W. Nuclear Instruments & Methods in Physics Research B, 2009, 267, 3197-3199.	1.4	24
156	First-principles study of the noble metal-doped BN layer. Journal of Applied Physics, 2011, 109, 084308.	2.5	24
157	Interplay between two-phase and solid solution reactions in high voltage spinel cathode material for lithium ion batteries. Journal of Power Sources, 2013, 242, 736-741.	7.8	24
158	Displacement damage and predicted non-ionizing energy loss in GaAs. Journal of Applied Physics, 2017, 121, .	2.5	24
159	Atomic-scale simulations of cascade overlap and damage evolution in silicon carbide. Journal of Materials Research, 2003, 18, 1877-1883.	2.6	23
160	First-principles calculation of defect formation energies and electronic properties in stannate pyrochlores. Journal of Applied Physics, 2008, 104, .	2.5	23
161	Yield, variance and spatial distribution of electronâ€“hole pairs in CsI. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2011, 652, 564-567.	1.6	23
162	Dislocation mechanism of deuterium retention in tungsten under plasma implantation. Journal of Physics Condensed Matter, 2014, 26, 395001.	1.8	23

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163	Atomistic study of hydrogen behavior around dislocations in Î± iron. Journal of Nuclear Materials, 2018, 510, 219-228.	2.7	23
164	Unraveling TM Migration Mechanisms in LiNi_{1/3}Mn_{1/3}Co_{1/3}O₂ by Modeling and Experimental Studies. Nano Letters, 2021, 21, 6875-6881.	9.1	23
165	Effects of interatomic potential on He bubble creation by cascades in Î±-iron. Journal of Applied Physics, 2008, 103, .	2.5	22
166	Hydrogenated Graphene Nanoflakes: Semiconductor to Half-Metal Transition and Remarkable Large Magnetism. Journal of Physical Chemistry C, 2012, 116, 5531-5537.	3.1	22
167	Ab initio study of stability and migration of point defects in copper-graphene layered composite. Journal of Alloys and Compounds, 2017, 692, 49-58.	5.5	22
168	Mechanisms for <100> interstitial dislocation loops to diffuse in BCC iron. Nature Communications, 2021, 12, 225.	12.8	22
169	Controlling electronic structures by irradiation in single-walled SiC nanotubes: a first-principles molecular dynamics study. Nanotechnology, 2009, 20, 075708.	2.6	21
170	First-principles study of the electronic properties of wurtzite, zinc-blende, and twinned InP nanowires. Nanotechnology, 2010, 21, 505709.	2.6	21
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