Fei Gao

List of Publications by Year
in descending order

373 papers	13,593 citations	25014 57 h-index	34964 98 g-index
375 all docs	375 docs citations	375 times ranked	11255 citing authors

#	Article	IF	Citations
1	10.1063/5.0072285.1. , 2022, , .		0
2	Ultrafast coherent control of a hole spin qubit in a germanium quantum dot. Nature Communications, 2022, 13, 206.	5.8	58
3	Abnormal radiation resistance via direct-amorphization-induced defect recovery in HgTe. Applied Physics Letters, 2022, 120, 012101.	1.5	0
4	Molecular dynamic simulations of displacement cascades in tungsten and tungstenâ€“rhenium alloys: Effects of grain boundary and/or Ïƒ phase. Journal of Nuclear Materials, 2022, 561, 153543.	1.3	7
5	Ab initio investigation of properties and mobility of helium defects in La2Sn2O7 pyrochlore. Nuclear Materials and Energy, 2022, 30, 101135.	0.6	0
6	Gate-Tunable Spin-Orbit Coupling in a Germanium Hole Double Quantum Dot. Physical Review Applied, 2022, 17, .	1.5	15
7	Strong interfacial coupling in vertical WSe2/WS2 heterostructure for high performance photodetection. Applied Physics Letters, 2022, 120, .	1.5	5
8	Manipulating Picosecond Photoresponse in van der Waals Heterostructure Photodetectors. Advanced Functional Materials, 2022, 32, .	7.8	6
9	Orientation dependence of shock-induced change of habit plane for the 1/2<111> dislocation loop and plasticity in tungsten. International Journal of Plasticity, 2022, 155, 103329.	4.1	11
10	Atomic modeling assessment of the interaction distance and effective bias for small defect clusters absorption at a void in BCC Fe. Journal of Nuclear Materials, 2022, 568, 153882.	1.3	1
11	Revealing the synergistic effect of invisible helium clusters in helium irradiation hardening in tungsten. Scripta Materialia, 2022, 219, 114850.	2.6	6
12	Physical properties and radiation tolerance of high-entropy pyrochlores Gd2(Ti0.25Zr0.25Sn0.25Hf0.25)2O7 and individual pyrochlores Gd2X2O7 (X= Ti, Zr, Sn, Hf) from first principles calculations. Scripta Materialia, 2022, 220, 114898.	2.6	5
13	Assessing Atomic-Phase Transitions and Ion Transport in Layered NaxNiO2 (x â‰ 0.67) Cathode Materials. Journal of Physical Chemistry C, 2021, 125, 4930-4937.	1.5	1
14	Atomistic study on helium-to-vacancy ratio of neutron irradiation induced helium bubbles during nucleation and growth in Î±-Fe. Nuclear Materials and Energy, 2021, 26, 100940.	0.6	1
15	Monte Carlo simulation of the passage of Î³-rays and Î±-particles in CsI. Nuclear Instruments & Methods in Physics Research B, 2021, 490, 25-33.	0.6	5
16	Atomistic simulation of displacement damage and effective nonionizing energy loss in InAs. Physical Review Materials, 2021, 5, .	0.9	5
17	Preface to the special issue on advanced materials for nuclear energy applications. Tungsten, 2021, 3, 1-2.	2.0	2
18	Ge/Si Quantum Wires for Quantum Computing. , 2021, , .		0

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19	Anisotropic g-Factor and Spinâ€“Orbit Field in a Germanium Hut Wire Double Quantum Dot. Nano Letters, 2021, 21, 3835-3842.	4.5	16
20	Defect capturing and charging dynamics and their effects on magneto-transport of electrons in quantum wells. Journal of Physics Condensed Matter, 2021, 33, 395304.	0.7	0
21	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.	4.5	23
22	Non-thermal melting of tungsten under intense electronic excitations. Acta Materialia, 2021, 216, 117158.	3.8	5
23	Formation mechanism of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>âŒ©</mml:mo><mml:mn>111</mml:mn><mml:mo> interstitial dislocation loops from irradiation-induced C15 clusters in tungsten. Physical Review Materials, 2021, 5, .	0.9	3
24	Perspectives on multiscale modelling and experiments to accelerate materials development for fusion. Journal of Nuclear Materials, 2021, 554, 153113.	1.3	37
25	Machine learning to predict aluminum segregation to magnesium grain boundaries. Scripta Materialia, 2021, 204, 114150.	2.6	18
26	Mechanisms for <100> interstitial dislocation loops to diffuse in BCC iron. Nature Communications, 2021, 12, 225.	5.8	22
27	Analytical bond-order potential for silver, palladium, ruthenium and iodine bulk diffusion in silicon carbide. Journal of Physics Condensed Matter, 2020, 32, 085702.	0.7	7
28	Atomistic simulations of the interaction between transmutation-produced Re and grain boundaries in tungsten. Computational Materials Science, 2020, 173, 109412.	1.4	9
29	Interatomic potentials and defect properties of Feâ€“Crâ€“Al alloys. Journal of Nuclear Materials, 2020, 541, 152421.	1.3	18
30	Study on the mechanism of helium platelets formation at low temperatures in SiC from the perspective of atomic diffusion. Journal of Nuclear Materials, 2020, 542, 152507.	1.3	9
31	Effect of H on the formation of vacancy dislocation loops in Î±-Fe. Journal of Nuclear Materials, 2020, 542, 152500.	1.3	8
32	Reaction heterogeneity in practical high-energy lithiumâ€“sulfur pouch cells. Energy and Environmental Science, 2020, 13, 3620-3632.	15.6	127
33	Molecular dynamics simulation of the diffusion of self-interstitial atoms and interstitial loops under temperature gradient field in tungsten. Journal of Applied Physics, 2020, 128, 065103.	1.1	5
34	Nanowires: Siteâ€Controlled Uniform Ge/Si Hut Wires with Electrically Tunable Spinâ€“Orbit Coupling (Adv. Mater. 16/2020). Advanced Materials, 2020, 32, 2070122.	11.1	0
35	Zero Field Splitting of Heavy-Hole States in Quantum Dots. Nano Letters, 2020, 20, 5201-5206.	4.5	12
36	Evolution of vacancy defects in heavy ion irradiated tungsten exposed to helium plasma. Journal of Nuclear Materials, 2020, 532, 152051.	1.3	19

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37	High Performance SiGe Body-On-Insulator (BOI) FinFET Fabricated on Bulk Si Substrate Using Ge Condensation Technique. IEEE Electron Device Letters, 2020, 41, 1280-1283.	2.2	9
38	Elucidating He-H assisted cavity evolution in alpha Cr under multiple ion beam irradiation. Scripta Materialia, 2020, 187, 291-295.	2.6	18
39	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. Acta Materialia, 2020, 196, 133-143.	3.8	124
40	Siteâ€Controlled Uniform Ge/Si Hut Wires with Electrically Tunable Spinâ€“Orbit Coupling. Advanced Materials, 2020, 32, e1906523.	11.1	40
41	Molecular dynamics simulations of radiation damage generation and dislocation loop evolution in Ni and binary Ni-based alloys. Computational Materials Science, 2020, 177, 109555.	1.4	18
42	Interatomic potentials of Wâ€“V and Wâ€“Mo binary systems for point defects studies. Journal of Nuclear Materials, 2020, 531, 152020.	1.3	18
43	Evaluation of tungsten interatomic potentials for radiation damage simulations. Tungsten, 2020, 2, 3-14.	2.0	12
44	Molecular dynamics simulation of the interactions between screw dislocation and stacking fault tetrahedron in Feâ€“10Niâ€“20Cr and Ni. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 075002.	0.8	3
45	Atomistic insights into the reaction mechanism of nanostructured LiI: Implications for rechargeable Li-I2 batteries. Energy Storage Materials, 2019, 17, 211-219.	9.5	10
46	Effect of vacancies on the nucleation of Cr precipitates at grain boundary in Î±-Fe. Canadian Journal of Physics, 2019, 97, 842-846.	0.4	0
47	Clustering and dislocation loop punching induced by different noble gas bubbles in tungsten: a molecular dynamics study. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 084002.	0.8	3
48	Reduction of defect generation and development of sinks at nanocluster boundary in oxide dispersion-strengthened steel. Journal of Applied Physics, 2019, 126, 084302.	1.1	1
49	Dopant Segregation Boosting Highâ€Voltage Cyclability of Layered Cathode for Sodium Ion Batteries. Advanced Materials, 2019, 31, e1904816.	11.1	89
50	Reveal the fast and charge-insensitive lattice diffusion of silver in cubic silicon carbide via first-principles calculations. Computational Materials Science, 2019, 170, 109190.	1.4	6
51	Modeling the effects of helium-vacancy clusters on the stress-strain response of a grain boundary in iron by a mechanistic finite element approach informed by molecular dynamics data. Journal of Nuclear Materials, 2019, 526, 151766.	1.3	3
52	Molecular dynamics simulations of high-energy radiation damage in W and Wâ€“Re alloys. Journal of Nuclear Materials, 2019, 524, 9-20.	1.3	36
53	Irradiation effects of medium-entropy alloy NiCoCr with and without pre-indentation. Journal of Nuclear Materials, 2019, 524, 60-66.	1.3	25
54	Molecular dynamics study of the material property changes induced by accumulated point defects in graphite. Nuclear Instruments & Methods in Physics Research B, 2019, 455, 52-56.	0.6	3

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55	Release of helium-related clusters through a nickelâ€“graphene interface: An atomistic study. Applied Surface Science, 2019, 487, 218-227.	3.1	8
56	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.	1.3	32
57	Ab initio study of interstitial helium clusters in 3C-SiC. Journal of Nuclear Materials, 2019, 521, 13-20.	1.3	12
58	Stability and physical properties tuning via interstitials chemical engineering of Zr5Sn3: a first-principles study. Journal of Materials Science, 2019, 54, 10284-10296.	1.7	4
59	First-Principles Assessment of the Structure and Stability of 15 Intrinsic Point Defects in Zinc-Blende Indium Arsenide. Crystals, 2019, 9, 48.	1.0	4
60	Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. Nuclear Fusion, 2019, 59, 076020.	1.6	13
61	Development of a Niâ€“Mo interatomic potential for irradiation simulation. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 045009.	0.8	4
62	Development of the interatomic potentials for W-Ta system. Computational Materials Science, 2019, 163, 91-99.	1.4	26
63	Proton irradiation of graphene: insights from atomistic modeling. Nanoscale, 2019, 11, 20754-20765.	2.8	20
64	Study of plasma induced nanostructure formation and surface morphology changes on tungsten and stainless steel at atmospheric pressure. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2019, 37, .	0.9	7
65	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. Journal of Alloys and Compounds, 2019, 775, 1184-1198.	2.8	30
66	Many-Body Theory of Proton-Generated Point Defects for Losses of Electron Energy and Photons in Quantum Wells. Physical Review Applied, 2018, 9, .	1.5	7
67	Coupling a Germanium Hut Wire Hole Quantum Dot to a Superconducting Microwave Resonator. Nano Letters, 2018, 18, 2091-2097.	4.5	36
68	Wetting characteristics of lithium droplet on iron surfaces in atomic scale: A molecular dynamics simulation. Computational Materials Science, 2018, 149, 435-441.	1.4	12
69	Revealing reaction mechanisms of nanoconfined Li2S: implications for lithiumâ€“sulfur batteries. Physical Chemistry Chemical Physics, 2018, 20, 11713-11721.	1.3	18
70	New interatomic potentials of W, Re and W-Re alloy for radiation defects. Journal of Nuclear Materials, 2018, 502, 141-153.	1.3	57
71	A first-principles investigation of the ScO₂ monolayer as the cathode material for alkali metal-ion batteries. Journal of Materials Chemistry A, 2018, 6, 3171-3180.	5.2	20
72	Atomic-Scale Simulation for Pseudometallic Defect-Generation Kinetics and Effective NIEL in GaN. IEEE Transactions on Nuclear Science, 2018, 65, 1108-1118.	1.2	17

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73	An ab initio study for probing iodization reactions on metallic anode surfaces of Liâ€“I₂ batteries. Journal of Materials Chemistry A, 2018, 6, 7807-7814.	5.2	11
74	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.	1.3	26
75	Dynamics of defect-loaded grain boundary under shear deformation in alpha iron. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 025006.	0.8	1
76	Shockwave generates < 100 > dislocation loops in bcc iron. Nature Communications, 2018, 9, 4880.	5.8	106
77	Does the Mgâ€“I₂ Battery Suffer Severe Shuttle Effect?. Journal of Physical Chemistry C, 2018, 122, 28518-28527.	1.5	9
78	A germanium hole spin qubit. Nature Communications, 2018, 9, 3902.	5.8	170
79	Effects of interstitial defects on stress-driven grain boundary migration in bcc tungsten. Journal of Nuclear Materials, 2018, 512, 246-251.	1.3	14
80	Ab initio study of the stability of intrinsic and extrinsic Ag point defects in 3C SiC. Journal of Nuclear Materials, 2018, 510, 596-602.	1.3	10
81	Self-healing mechanism of irradiation defects in nickelâ€“graphene nanocomposite: An energetic and kinetic perspective. Journal of Alloys and Compounds, 2018, 765, 253-263.	2.8	27
82	Interstitial migration behavior and defect evolution in ion irradiated pure nickel and Ni-xFe binary alloys. Journal of Nuclear Materials, 2018, 509, 237-244.	1.3	34
83	Energetics and structures of hydrogen-vacancy clusters in tungsten based on genetic algorithm. Science China: Physics, Mechanics and Astronomy, 2018, 61, 1.	2.0	9
84	Measuring the complex admittance and tunneling rate of a germanium hut wire hole quantum dot. Journal of Applied Physics, 2018, 123, 174305.	1.1	3
85	Atomistic study of hydrogen behavior around dislocations in Î± iron. Journal of Nuclear Materials, 2018, 510, 219-228.	1.3	23
86	Theoretical prediction of LiScO₂ nanosheets as a cathode material for Liâ€“O₂ batteries. Physical Chemistry Chemical Physics, 2018, 20, 22351-22358.	1.3	7
87	Enhanced void swelling in NiCoFeCrPd high-entropy alloy by indentation-induced dislocations. Materials Research Letters, 2018, 6, 584-591.	4.1	46
88	Effect of neon on the hydrogen behaviors in tungsten: AÂfirst-principles study. Journal of Nuclear Materials, 2018, 510, 492-498.	1.3	3
89	Modified analytic embedded atom method potential for chromium. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 065001.	0.8	4
90	Plasma Induced Nanostructures on the Surface of Tungsten Anode in Atmospheric Pressure Glow. , 2018, , .		0

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91	Microscopic theory for point-defect effects on photon absorption in quantum-well systems. , 2018, , .		0
92	Atomic-level based non-ionizing energy loss: an application to GaAs and GaN semiconductor materials. , 2018, , .		1
93	Long-time atomistic dynamics through a new self-adaptive accelerated molecular dynamics method. Journal of Physics Condensed Matter, 2017, 29, 145201.	0.7	10
94	Radiation-induced segregation on defect clusters in single-phase concentrated solid-solution alloys. Acta Materialia, 2017, 127, 98-107.	3.8	212
95	Enhanced formation of <1 0 0> and <1 1 1> interstitial loops by helium clustering in bcc iron. Materials Letters, 2017, 190, 260-262.	1.3	6
96	Molecular Dynamics Study: Effects of He Bubble and Cr Precipitate on Tensile Deformation of Grain Boundaries in $alpha$ -Fe. IEEE Transactions on Plasma Science, 2017, 45, 289-293.	0.6	13
97	Evolution of nanoscale interstitial dislocation loops under coupling effect of stress and temperature. Scripta Materialia, 2017, 136, 64-67.	2.6	13
98	Computational simulation of threshold displacement energies of GaAs. Journal of Materials Research, 2017, 32, 1555-1562.	1.2	20
99	Heâ€“V cluster nucleation and growth in Î±-Fe grain boundaries. Acta Materialia, 2017, 124, 544-555.	3.8	27
100	Measuring hole spin states of single quantum dot in germanium hut wire. Applied Physics Letters, 2017, 110, .	1.5	19
101	Low energy ionâ€solid interactions and chemistry effects in a series of pyrochlores. Journal of the American Ceramic Society, 2017, 100, 3132-3144.	1.9	7
102	Displacement damage and predicted non-ionizing energy loss in GaAs. Journal of Applied Physics, 2017, 121, .	1.1	24
103	Enhanced Radiation-tolerant Oxide Dispersion Strengthened Steel and its Microstructure Evolution under Helium-implantation and Heavy-ion Irradiation. Scientific Reports, 2017, 7, 40343.	1.6	34
104	Embedded-atom method potential for modeling hydrogen and hydrogen-defect interaction in tungsten. Journal of Physics Condensed Matter, 2017, 29, 435401.	0.7	26
105	New understanding of nano-scale interstitial dislocation loops in BCC iron. Journal of Physics Condensed Matter, 2017, 29, 455301.	0.7	16
106	Helium nano-bubble bursting near the nickel surface. Chinese Physics B, 2017, 26, 113401.	0.7	3
107	High performance computing for advanced modeling and simulation of materials. Computer Physics Communications, 2017, 211, 1.	3.0	7
108	Ab initio study of stability and migration of point defects in copper-graphene layered composite. Journal of Alloys and Compounds, 2017, 692, 49-58.	2.8	22

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109	Monte Carlo simulation of electron thermalization in scintillator materials: Implications for scintillator nonproportionality. Journal of Applied Physics, 2017, 122, .	1.1	16
110	Anisotropic Migration of Defects under Strain Effect in BCC Iron. Chinese Physics Letters, 2017, 34, 076102.	1.3	2
111	An Isotropic Empirical Intermolecular Potential for Solid H 2 and D 2 : A Classical Molecular Calculation. Chinese Physics Letters, 2017, 34, 123401.	1.3	0
112	Molecular dynamics simulation of low-energy recoil events in titanate pyrochlores. RSC Advances, 2017, 7, 35403-35410.	1.7	6
113	Atomistic Conversion Reaction Mechanism of WO₃ in Secondary Ion Batteries of Li, Na, and Ca. Angewandte Chemie - International Edition, 2016, 55, 6244-6247.	7.2	86
114	Crossover from disordered to core-shell structures of nano-oxide Y2O3 dispersed particles in Fe. Applied Physics Letters, 2016, 109, .	1.5	15
115	Modeling and Simulation of Primary Damage and Structure Evolution in Ceramics and Metals. EPJ Web of Conferences, 2016, 115, 02001.	0.1	1
116	Enhancing radiation tolerance by controlling defect mobility and migration pathways in multicomponent single-phase alloys. Nature Communications, 2016, 7, 13564.	5.8	533
117	Evidencing the existence of exciting half-metallicity in two-dimensional TiCl3 and VCl3 sheets. Scientific Reports, 2016, 6, 19407.	1.6	76
118	Shear-coupled grain boundary migration assisted by unusual atomic shuffling. Scientific Reports, 2016, 6, 23602.	1.6	18
119	Molecular dynamics simulation of the structural, elastic, and thermal properties of pyrochlores. RSC Advances, 2016, 6, 41410-41419.	1.7	25
120	Analytical interactomic potential for a molybdenumâ€“erbium system. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 045018.	0.8	2
121	Spontaneous ripple formation in phosphorene: electronic properties and possible applications. Nanoscale, 2016, 8, 11827-11833.	2.8	11
122	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.	1.7	30
123	Energetics of vacancy segregation to [100] symmetric tilt grain boundaries in bcc tungsten. Scientific Reports, 2016, 6, 36955.	1.6	31
124	Atomistic insights into shear-coupled grain boundary migration in bcc tungsten. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2016, 677, 20-28.	2.6	14
125	Carrier-Multiplication-Induced Structural Change during Ultrafast Carrier Relaxation and Nonthermal Phase Transition in Semiconductors. Physical Review Letters, 2016, 117, 126402.	2.9	29
126	A first-principles study of the avalanche pressure of alpha zirconium. RSC Advances, 2016, 6, 72551-72558.	1.7	1

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127	Atomistic Conversion Reaction Mechanism of WO₃ in Secondary Ion Batteries of Li, Na, and Ca. Angewandte Chemie, 2016, 128, 6352-6355.	1.6	21
128	First-principles search for efficient activators for LaI3. Journal of Luminescence, 2016, 176, 227-234.	1.5	11
129	Grain boundary resistance to amorphization of nanocrystalline silicon carbide. Scientific Reports, 2015, 5, 16602.	1.6	11
130	Multi-Timescale Microscopic Theory for Radiation Degradation of Electronic and Optoelectronic Devices. Space Science International, 2015, 3, 3-27.	0.3	2
131	Microscopic model for studying radiation degradation of electron transport and photodetection devices. Proceedings of SPIE, 2015, , .	0.8	0
132	Molecular-confinement of polysulfides within mesoscale electrodes for the practical application of lithium sulfur batteries. Nano Energy, 2015, 13, 267-274.	8.2	50
133	Probing the Degradation Mechanism of Li₂MnO₃ Cathode for Li-Ion Batteries. Chemistry of Materials, 2015, 27, 975-982.	3.2	130
134	â€œH₂ spongeâ€• pressure as a means for reversible high-capacity hydrogen storage in nanoporous Ca-intercalated covalent organic frameworks. Nanoscale, 2015, 7, 6319-6324.	2.8	12
135	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.	3.8	54
136	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. Journal of Nuclear Materials, 2015, 467, 398-405.	1.3	16
137	Interplay between intrinsic point defects and low-angle grain boundary in bcc tungsten: effects of local stress field. Journal of Physics Condensed Matter, 2015, 27, 255007.	0.7	18
138	Nucleation of Cr precipitates in Feâ€“Cr alloy under irradiation. Computational Materials Science, 2015, 101, 293-300.	1.4	14
139	Effect of hydrogen on grain boundary migration in tungsten. Science China: Physics, Mechanics and Astronomy, 2015, 58, 1-9.	2.0	11
140	Calculation of energy relaxation rates of fast particles by phonons in crystals. Physical Review B, 2015, 91, .	1.1	12
141	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.	4.5	261
142	Atomistic simulations of helium clustering and grain boundary reconstruction in alpha-iron. Acta Materialia, 2015, 82, 275-286.	3.8	36
143	Dislocation-accelerated void formation under irradiation in zirconium. Acta Materialia, 2015, 82, 94-99.	3.8	26
144	Anab initio-based Erâ€“He interatomic potential in hcp Er. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 065009.	0.8	3

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145	Interplay between atomic disorder, lattice swelling, and defect energy in ion-irradiation-induced amorphization of SiC. Physical Review B, 2014, 90, .	1.1	36
146	Theory of suppressing avalanche process of carrier in short pulse laser irradiated dielectrics. Journal of Applied Physics, 2014, 115, 203112.	1.1	3
147	Ab initio calculations of mechanical properties in Î²-MH2â^'xHex (M = Er, Sc). European Physical Journal B, 2014, 87, 1.	0.6	2
148	Energetics of Defects on Graphene through Fluorination. ChemSusChem, 2014, 7, 1295-1300.	3.6	10
149	Precipitates of Cr at Î£3 <110> {112} GB in Î±-Fe. Materials Research Society Symposia Proceedings, 2014, 1645, 1.	0.1	0
150	Cu Segregation at Î£ 5 Symmetrical Grain Boundary in Î± -Fe: Atomic-Level Simulations. Chinese Physics Letters, 2014, 31, 096801.	1.3	4
151	Radiation response of inorganic scintillators: insights from Monte Carlo simulations. Proceedings of SPIE, 2014, , .	0.8	3
152	Modeling radiation damage near grain boundary in helium-doped Î±-iron. Nuclear Instruments & Methods in Physics Research B, 2014, 332, 426-431.	0.6	9
153	Kinetic Monte Carlo Simulations of Scintillation Processes in NaI(Tl). IEEE Transactions on Nuclear Science, 2014, 61, 860-869.	1.2	12
154	Binding of HenV clusters to Î±-Fe grain boundaries. Journal of Applied Physics, 2014, 115, .	1.1	16
155	Binding energetics of substitutional and interstitial helium and di-helium defects with grain boundary structure in Î±-Fe. Journal of Applied Physics, 2014, 115, .	1.1	31
156	Molecular dynamics simulation of helium cluster diffusion and bubble formation in bulk tungsten. Journal of Nuclear Materials, 2014, 455, 544-548.	1.3	58
157	Migration of defect clusters and xenon-vacancy clusters in uranium dioxide. International Journal of Modern Physics B, 2014, 28, 1450120.	1.0	2
158	Dislocation mechanism of deuterium retention in tungsten under plasma implantation. Journal of Physics Condensed Matter, 2014, 26, 395001.	0.7	23
159	Understanding the presence of vacancy clusters in ZnO from a kinetic perspective. Applied Physics Letters, 2014, 104, 252101.	1.5	34
160	Lewis Acidâ€"Base Interactions between Polysulfides and Metal Organic Framework in Lithium Sulfur Batteries. Nano Letters, 2014, 14, 2345-2352.	4.5	623
161	Structural evolution of NiAu nanoparticles under ambient conditions directly revealed by atom-resolved imaging combined with DFT simulation. Nanoscale, 2014, 6, 12898-12904.	2.8	9
162	Prediction of thermal conductivity for irradiated SiC/SiC composites by informing continuum models with molecular dynamics data. Journal of Nuclear Materials, 2014, 448, 364-372.	1.3	8

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163	Molecular Dynamics Simulation of Thermodynamic Properties in Uranium Dioxide. Nuclear Science and Engineering, 2014, 176, 360-369.	0.5	0
164	Evidencing the existence of intrinsic half-metallicity and ferromagnetism in zigzag gallium sulfide nanoribbons. Scientific Reports, 2014, 4, 5773.	1.6	8
165	Pressure effect on stabilities of self-Interstitials in HCP-Zirconium. Scientific Reports, 2014, 4, 5735.	1.6	18
166	Effects of surface defects on two-dimensional electron gas at NdAlO3/SrTiO3 interface. Scientific Reports, 2014, 4, 5477.	1.6	15
167	First principles prediction of nitrogen-doped carbon nanotubes as a high-performance cathode for Liâ€“S batteries. RSC Advances, 2013, 3, 16775.	1.7	44
168	Transition Metal Adsorption Promotes Patterning and Doping of Graphene by Electron Irradiation. Journal of Physical Chemistry C, 2013, 117, 17644-17649.	1.5	9
169	Three-dimensional metal-intercalated covalent organic frameworks for near-ambient energy storage. Scientific Reports, 2013, 3, 1882.	1.6	31
170	Mechanical and electronic properties of A1â^'xBxHy (A and B=Ti, Zr, Hf) hydride alloys: A first-principles study. Journal of Alloys and Compounds, 2013, 581, 404-412.	2.8	5
171	Electron-Rich Driven Electrochemical Solid-State Amorphization in Liâ€“Si Alloys. Nano Letters, 2013, 13, 4511-4516.	4.5	51
172	Role of cation choice in the radiation tolerance of pyrochlores. RSC Advances, 2013, 3, 2901.	1.7	19
173	Excited state electronic properties of sodium iodide and cesium iodide. Journal of Luminescence, 2013, 137, 121-131.	1.5	13
174	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.	3.3	32
175	Ab initio study of He point defects in fcc Auâ€“Ag alloys. Journal of Alloys and Compounds, 2013, 557, 5-10.	2.8	6
176	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.	0.6	50
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