Fei Gao

List of Publications by Year in Descending Order

358 papers	10,915 citations	53 h-index	89 g-index
375 ext. papers	12,302 ext. citations	4.2 avg, IF	6.28 L-index

#	Paper	IF	Citations
358	Molecular dynamic simulations of displacement cascades in tungsten and tungsten□henium alloys: Effects of grain boundary and/or □phase. *Journal of Nuclear Materials*, **2022**, 561, 153543	3.3	1
357	Ab initio investigation of properties and mobility of helium defects in La2Sn2O7 pyrochlore. *Nuclear Materials and Energy*, **2022**, 30, 101135	2.1	
356	Ultrafast coherent control of a hole spin qubit in a germanium quantum dot.. *Nature Communications*, **2022**, 13, 206	17.4	5
355	Abnormal radiation resistance via direct-amorphization-induced defect recovery in HgTe. *Applied Physics Letters*, **2022**, 120, 012101	3.4	
354	Strong interfacial coupling in vertical WSe2/WS2 heterostructure for high performance photodetection. *Applied Physics Letters*, **2022**, 120, 181108	3.4	0
353	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	7.6	0
352	Atomistic study on helium-to-vacancy ratio of neutron irradiation induced helium bubbles during nucleation and growth in □Fe. *Nuclear Materials and Energy*, **2021**, 26, 100940	2.1	
351	Monte Carlo simulation of the passage of □rays and □particles in CsI. *Nuclear Instruments & Methods in Physics Research B*, **2021**, 490, 25-33	1.2	0
350	Atomistic simulation of displacement damage and effective nonionizing energy loss in InAs. *Physical Review Materials*, **2021**, 5,	3.2	2
349	Anisotropic -Factor and Spin-Orbit Field in a Germanium Hut Wire Double Quantum Dot. *Nano Letters*, **2021**, 21, 3835-3842	11.5	5
348	Assessing Atomic-Phase Transitions and Ion Transport in Layered NaxNiO2 (x □0.67) Cathode Materials. *Journal of Physical Chemistry C*, **2021**, 125, 4930-4937	3.8	
347	Unraveling TM Migration Mechanisms in LiNiMnCoO by Modeling and Experimental Studies. *Nano Letters*, **2021**, 21, 6875-6881	11.5	6
346	Non-thermal melting of tungsten under intense electronic excitations. *Acta Materialia*, **2021**, 216, 117158	8.4	2
345	Perspectives on multiscale modelling and experiments to accelerate materials development for fusion. *Journal of Nuclear Materials*, **2021**, 554, 153113	3.3	7
344	Machine learning to predict aluminum segregation to magnesium grain boundaries. *Scripta Materialia*, **2021**, 204, 114150	5.6	2
343	Mechanisms for interstitial dislocation loops to diffuse in BCC iron. *Nature Communications*, **2021**, 12, 225	17.4	10
342	Nanowires: Site-Controlled Uniform Ge/Si Hut Wires with Electrically Tunable Spin□Orbit Coupling (Adv. Mater. 16/2020). *Advanced Materials*, **2020**, 32, 2070122	24	

341	Zero Field Splitting of Heavy-Hole States in Quantum Dots. *Nano Letters*, **2020**, 20, 5201-5206	11.5	4
340	Evolution of vacancy defects in heavy ion irradiated tungsten exposed to helium plasma. *Journal of Nuclear Materials*, **2020**, 532, 152051	3.3	8
339	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	4.4	2
338	Elucidating He-H assisted cavity evolution in alpha Cr under multiple ion beam irradiation. *Scripta Materialia*, **2020**, 187, 291-295	5.6	7
337	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. *Acta Materialia*, **2020**, 196, 133-143	8.4	45
336	Site-Controlled Uniform Ge/Si Hut Wires with Electrically Tunable Spin-Orbit Coupling. *Advanced Materials*, **2020**, 32, e1906523	24	14
335	Molecular dynamics simulations of radiation damage generation and dislocation loop evolution in Ni and binary Ni-based alloys. *Computational Materials Science*, **2020**, 177, 109555	3.2	5
334	Interatomic potentials of W□V and W□Mo binary systems for point defects studies. *Journal of Nuclear Materials*, **2020**, 531, 152020	3.3	5
333	Evaluation of tungsten interatomic potentials for radiation damage simulations. *Tungsten*, **2020**, 2, 3-14	4.6	3
332	Molecular dynamics simulation of the interactions between screw dislocation and stacking fault tetrahedron in Fe□10Ni□20Cr and Ni. *Modelling and Simulation in Materials Science and Engineering*, **2020**, 28, 075002	2	2
331	Analytical bond-order potential for silver, palladium, ruthenium and iodine bulk diffusion in silicon carbide. *Journal of Physics Condensed Matter*, **2020**, 32, 085702	1.8	3
330	Atomistic simulations of the interaction between transmutation-produced Re and grain boundaries in tungsten. *Computational Materials Science*, **2020**, 173, 109412	3.2	4
329	Interatomic potentials and defect properties of Fe□Cr□Al alloys. *Journal of Nuclear Materials*, **2020**, 541, 152421	3.3	6
328	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	3.3	3
327	Effect of H on the formation of vacancy dislocation loops in □Fe. *Journal of Nuclear Materials*, **2020**, 542, 152500	3.3	2
326	Reaction heterogeneity in practical high-energy lithium□sulfur pouch cells. *Energy and Environmental Science*, **2020**, 13, 3620-3632	35.4	59
325	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	2.5	4
324	Reveal the fast and charge-insensitive lattice diffusion of silver in cubic silicon carbide via first-principles calculations. *Computational Materials Science*, **2019**, 170, 109190	3.2	5

323	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	3.3	3
322	Molecular dynamics simulations of high-energy radiation damage in W and W□Re alloys. *Journal of Nuclear Materials*, **2019**, 524, 9-20	3.3	12
321	Irradiation effects of medium-entropy alloy NiCoCr with and without pre-indentation. *Journal of Nuclear Materials*, **2019**, 524, 60-66	3.3	12
320	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	1.2	3
319	Release of helium-related clusters through a nickel□graphene interface: An atomistic study. *Applied Surface Science*, **2019**, 487, 218-227	6.7	3
318	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	3.3	16
317	Ab initio study of interstitial helium clusters in 3C-SiC. *Journal of Nuclear Materials*, **2019**, 521, 13-20	3.3	9
316	Stability and physical properties tuning via interstitials chemical engineering of Zr5Sn3: a first-principles study. *Journal of Materials Science*, **2019**, 54, 10284-10296	4.3	1
315	First-Principles Assessment of the Structure and Stability of 15 Intrinsic Point Defects in Zinc-Blende Indium Arsenide. *Crystals*, **2019**, 9, 48	2.3	2
314	Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. *Nuclear Fusion*, **2019**, 59, 076020	3.3	7
313	Development of a Ni□Mo interatomic potential for irradiation simulation. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 045009	2	4
312	Development of the interatomic potentials for W-Ta system. *Computational Materials Science*, **2019**, 163, 91-99	3.2	10
311	Atomistic insights into the reaction mechanism of nanostructured LiI: Implications for rechargeable Li-I2 batteries. *Energy Storage Materials*, **2019**, 17, 211-219	19.4	7
310	Effect of vacancies on the nucleation of Cr precipitates at grain boundary in □Fe. *Canadian Journal of Physics*, **2019**, 97, 842-846	1.1	
309	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	2	0
308	Reduction of defect generation and development of sinks at nanocluster boundary in oxide dispersion-strengthened steel. *Journal of Applied Physics*, **2019**, 126, 084302	2.5	0
307	Dopant Segregation Boosting High-Voltage Cyclability of Layered Cathode for Sodium Ion Batteries. *Advanced Materials*, **2019**, 31, e1904816	24	46
306	Proton irradiation of graphene: insights from atomistic modeling. *Nanoscale*, **2019**, 11, 20754-20765	7.7	10

305	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, 011301	2.9	4
304	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. *Journal of Alloys and Compounds*, **2019**, 775, 1184-1198	5.7	17
303	Many-Body Theory of Proton-Generated Point Defects for Losses of Electron Energy and Photons in Quantum Wells. *Physical Review Applied*, **2018**, 9,	4.3	2
302	Coupling a Germanium Hut Wire Hole Quantum Dot to a Superconducting Microwave Resonator. *Nano Letters*, **2018**, 18, 2091-2097	11.5	24
301	Wetting characteristics of lithium droplet on iron surfaces in atomic scale: A molecular dynamics simulation. *Computational Materials Science*, **2018**, 149, 435-441	3.2	2
300	Revealing reaction mechanisms of nanoconfined LiS: implications for lithium-sulfur batteries. *Physical Chemistry Chemical Physics*, **2018**, 20, 11713-11721	3.6	18
299	New interatomic potentials of W, Re and W-Re alloy for radiation defects. *Journal of Nuclear Materials*, **2018**, 502, 141-153	3.3	35
298	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	13	15
297	Atomic-Scale Simulation for Pseudometallic Defect-Generation Kinetics and Effective NIEL in GaN. *IEEE Transactions on Nuclear Science*, **2018**, 65, 1108-1118	1.7	9
296	An ab initio study for probing iodization reactions on metallic anode surfaces of Li□2 batteries. *Journal of Materials Chemistry A*, **2018**, 6, 7807-7814	13	6
295	Interstitial migration behavior and defect evolution in ion irradiated pure nickel and Ni-xFe binary alloys. *Journal of Nuclear Materials*, **2018**, 509, 237-244	3.3	20
294	Energetics and structures of hydrogen-vacancy clusters in tungsten based on genetic algorithm. *Science China: Physics, Mechanics and Astronomy*, **2018**, 61, 1	3.6	9
293	Measuring the complex admittance and tunneling rate of a germanium hut wire hole quantum dot. *Journal of Applied Physics*, **2018**, 123, 174305	2.5	1
292	Atomistic study of hydrogen behavior around dislocations in □ron. *Journal of Nuclear Materials*, **2018**, 510, 219-228	3.3	10
291	Theoretical prediction of LiScO nanosheets as a cathode material for Li-O batteries. *Physical Chemistry Chemical Physics*, **2018**, 20, 22351-22358	3.6	6
290	Enhanced void swelling in NiCoFeCrPd high-entropy alloy by indentation-induced dislocations. *Materials Research Letters*, **2018**, 6, 584-591	7.4	27
289	Effect of neon on the hydrogen behaviors in tungsten: A first-principles study. *Journal of Nuclear Materials*, **2018**, 510, 492-498	3.3	2
288	Modified analytic embedded atom method potential for chromium. *Modelling and Simulation in Materials Science and Engineering*, **2018**, 26, 065001	2	2

287	A first-principles study of the structural, mechanical and electronic properties of precipitates of AlCu in Al-Cu alloys. *Physical Chemistry Chemical Physics*, **2018**, 20, 967-976	3.6	15
286	Dynamics of defect-loaded grain boundary under shear deformation in alpha iron. *Modelling and Simulation in Materials Science and Engineering*, **2018**, 26, 025006	2	0
285	Shockwave generates dislocation loops in bcc iron. *Nature Communications*, **2018**, 9, 4880	17.4	74
284	Does the Mg□2 Battery Suffer Severe Shuttle Effect?. *Journal of Physical Chemistry C*, **2018**, 122, 28518-28527	3.3	3
283	A germanium hole spin qubit. *Nature Communications*, **2018**, 9, 3902	17.4	84
282	Effects of interstitial defects on stress-driven grain boundary migration in bcc tungsten. *Journal of Nuclear Materials*, **2018**, 512, 246-251	3.3	9
281	Ab initio study of the stability of intrinsic and extrinsic Ag point defects in 3CSiC. *Journal of Nuclear Materials*, **2018**, 510, 596-602	3.3	7
280	Self-healing mechanism of irradiation defects in nickel□graphene nanocomposite: An energetic and kinetic perspective. *Journal of Alloys and Compounds*, **2018**, 765, 253-263	5.7	18
279	Long-time atomistic dynamics through a new self-adaptive accelerated molecular dynamics method. *Journal of Physics Condensed Matter*, **2017**, 29, 145201	1.8	8
278	Radiation-induced segregation on defect clusters in single-phase concentrated solid-solution alloys. *Acta Materialia*, **2017**, 127, 98-107	8.4	128
277	Enhanced formation of and interstitial loops by helium clustering in bcc iron. *Materials Letters*, **2017**, 190, 260-262	3.3	6
276	. *IEEE Transactions on Plasma Science*, **2017**, 45, 289-293	1.3	7
275	Evolution of nanoscale interstitial dislocation loops under coupling effect of stress and temperature. *Scripta Materialia*, **2017**, 136, 64-67	5.6	8
274	Computational simulation of threshold displacement energies of GaAs. *Journal of Materials Research*, **2017**, 32, 1555-1562	2.5	11
273	He□V cluster nucleation and growth in □-Fe grain boundaries. *Acta Materialia*, **2017**, 124, 544-555	8.4	22
272	Measuring hole spin states of single quantum dot in germanium hut wire. *Applied Physics Letters*, **2017**, 110, 133105	3.4	16
271	Low energy ion-solid interactions and chemistry effects in a series of pyrochlores. *Journal of the American Ceramic Society*, **2017**, 100, 3132-3144	3.8	2
270	Displacement damage and predicted non-ionizing energy loss in GaAs. *Journal of Applied Physics*, **2017**, 121, 095104	2.5	13

269	Enhanced Radiation-tolerant Oxide Dispersion Strengthened Steel and its Microstructure Evolution under Helium-implantation and Heavy-ion Irradiation. *Scientific Reports*, **2017**, 7, 40343	4.9	27
268	Anisotropic Migration of Defects under Strain Effect in BCC Iron. *Chinese Physics Letters*, **2017**, 34, 076102	1.28	2
267	An Isotropic Empirical Intermolecular Potential for Solid H 2 and D 2 : A Classical Molecular Calculation. *Chinese Physics Letters*, **2017**, 34, 123401	1.8	
266	Embedded-atom method potential for modeling hydrogen and hydrogen-defect interaction in tungsten. *Journal of Physics Condensed Matter*, **2017**, 29, 435401	1.8	13
265	New understanding of nano-scale interstitial dislocation loops in BCC iron. *Journal of Physics Condensed Matter*, **2017**, 29, 455301	1.8	11
264	Helium nano-bubble bursting near the nickel surface. *Chinese Physics B*, **2017**, 26, 113401	1.2	1
263	High performance computing for advanced modeling and simulation of materials. *Computer Physics Communications*, **2017**, 211, 1	4.2	7
262	Ab initio study of stability and migration of point defects in copper-graphene layered composite. *Journal of Alloys and Compounds*, **2017**, 692, 49-58	5.7	17
261	Monte Carlo simulation of electron thermalization in scintillator materials: Implications for scintillator nonproportionality. *Journal of Applied Physics*, **2017**, 122, 234504	2.5	12
260	Molecular dynamics simulation of low-energy recoil events in titanate pyrochlores. *RSC Advances*, **2017**, 7, 35403-35410	3.7	3
259	Synthesis of CN dual-doped Cr2O3 visible light-driven photocatalysts derived from metalorganic framework (MOF) for cyclohexane oxidation. *RSC Advances*, **2016**, 6, 84871-84881	3.7	25
258	Energetics of vacancy segregation to [100] symmetric tilt grain boundaries in bcc tungsten. *Scientific Reports*, **2016**, 6, 36955	4.9	23
257	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	5.3	10
256	Carrier-Multiplication-Induced Structural Change during Ultrafast Carrier Relaxation and Nonthermal Phase Transition in Semiconductors. *Physical Review Letters*, **2016**, 117, 126402	7.4	20
255	A first-principles study of the avalanche pressure of alpha zirconium. *RSC Advances*, **2016**, 6, 72551-72558	3.7	1
254	Atomistic Conversion Reaction Mechanism of WO3 in Secondary Ion Batteries of Li, Na, and Ca. *Angewandte Chemie*, **2016**, 128, 6352-6355	3.6	13
253	First-principles search for efficient activators for LaI3. *Journal of Luminescence*, **2016**, 176, 227-234	3.8	9
252	Atomistic Conversion Reaction Mechanism of WO3 in Secondary Ion Batteries of Li, Na, and Ca. *Angewandte Chemie - International Edition*, **2016**, 55, 6244-7	16.4	70

251	Crossover from disordered to core-shell structures of nano-oxide Y2O3 dispersed particles in Fe. *Applied Physics Letters*, **2016**, 109, 031911	3.4	10
250	Enhancing radiation tolerance by controlling defect mobility and migration pathways in multicomponent single-phase alloys. *Nature Communications*, **2016**, 7, 13564	17.4	336
249	Evidencing the existence of exciting half-metallicity in two-dimensional TiCl3 and VCl3 sheets. *Scientific Reports*, **2016**, 6, 19407	4.9	60
248	Shear-coupled grain boundary migration assisted by unusual atomic shuffling. *Scientific Reports*, **2016**, 6, 23602	4.9	11
247	Molecular dynamics simulation of the structural, elastic, and thermal properties of pyrochlores. *RSC Advances*, **2016**, 6, 41410-41419	3.7	18
246	Analytical interactomic potential for a molybdenum□rbium system. *Modelling and Simulation in Materials Science and Engineering*, **2016**, 24, 045018	2	2
245	Spontaneous ripple formation in phosphorene: electronic properties and possible applications. *Nanoscale*, **2016**, 8, 11827-33	7.7	9
244	Probing the Degradation Mechanism of Li2MnO3 Cathode for Li-Ion Batteries. *Chemistry of Materials*, **2015**, 27, 975-982	9.6	107
243	"H□sponge": pressure as a means for reversible high-capacity hydrogen storage in nanoporous Ca-intercalated covalent organic frameworks. *Nanoscale*, **2015**, 7, 6319-24	7.7	11
242	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	8.4	35
241	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. *Journal of Nuclear Materials*, **2015**, 467, 398-405	3.3	13
240	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	1.8	12
239	Nucleation of Cr precipitates in Fe□Cr alloy under irradiation. *Computational Materials Science*, **2015**, 101, 293-300	3.2	11
238	Effect of hydrogen on grain boundary migration in tungsten. *Science China: Physics, Mechanics and Astronomy*, **2015**, 58, 1-9	3.6	9
237	Calculation of energy relaxation rates of fast particles by phonons in crystals. *Physical Review B*, **2015**, 91,	3.3	9
236	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, 514-22	11.5	213
235	Atomistic simulations of helium clustering and grain boundary reconstruction in alpha-iron. *Acta Materialia*, **2015**, 82, 275-286	8.4	33
234	Dislocation-accelerated void formation under irradiation in zirconium. *Acta Materialia*, **2015**, 82, 94-99	8.4	24

233	Grain boundary resistance to amorphization of nanocrystalline silicon carbide. *Scientific Reports*, **2015**, 5, 16602	4.9	10
232	Multi-Timescale Microscopic Theory for Radiation Degradation of Electronic and Optoelectronic Devices. *Space Science International*, **2015**, 3, 3-27		1
231	Molecular-confinement of polysulfides within mesoscale electrodes for the practical application of lithium sulfur batteries. *Nano Energy*, **2015**, 13, 267-274	17.1	43
230	Evidencing the existence of intrinsic half-metallicity and ferromagnetism in zigzag gallium sulfide nanoribbons. *Scientific Reports*, **2014**, 4, 5773	4.9	7
229	Pressure effect on stabilities of self-interstitials in HCP-zirconium. *Scientific Reports*, **2014**, 4, 5735	4.9	11
228	Effects of surface defects on two-dimensional electron gas at NdAlO3/SrTiO3 interface. *Scientific Reports*, **2014**, 4, 5477	4.9	12
227	Kinetic Monte Carlo Simulations of Scintillation Processes in NaI(Tl). *IEEE Transactions on Nuclear Science*, **2014**, 61, 860-869	1.7	10
226	Binding of HenV clusters to □Fe grain boundaries. *Journal of Applied Physics*, **2014**, 115, 233501	2.5	15
225	Binding energetics of substitutional and interstitial helium and di-helium defects with grain boundary structure in □Fe. *Journal of Applied Physics*, **2014**, 115, 033503	2.5	26
224	Molecular dynamics simulation of helium cluster diffusion and bubble formation in bulk tungsten. *Journal of Nuclear Materials*, **2014**, 455, 544-548	3.3	46
223	Migration of defect clusters and xenon-vacancy clusters in uranium dioxide. *International Journal of Modern Physics B*, **2014**, 28, 1450120	1.1	2
222	Dislocation mechanism of deuterium retention in tungsten under plasma implantation. *Journal of Physics Condensed Matter*, **2014**, 26, 395001	1.8	22
221	Understanding the presence of vacancy clusters in ZnO from a kinetic perspective. *Applied Physics Letters*, **2014**, 104, 252101	3.4	33
220	Lewis acid-base interactions between polysulfides and metal organic framework in lithium sulfur batteries. *Nano Letters*, **2014**, 14, 2345-52	11.5	529
219	Structural evolution of NiAu nanoparticles under ambient conditions directly revealed by atom-resolved imaging combined with DFT simulation. *Nanoscale*, **2014**, 6, 12898-904	7.7	8
218	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	3.3	8
217	Molecular Dynamics Simulation of Thermodynamic Properties in Uranium Dioxide. *Nuclear Science and Engineering*, **2014**, 176, 360-369	1.2	
216	Anab initio-based Er□e interatomic potential in hcp Er. *Modelling and Simulation in Materials Science and Engineering*, **2014**, 22, 065009	2	3

215	Interplay between atomic disorder, lattice swelling, and defect energy in ion-irradiation-induced amorphization of SiC. *Physical Review B*, **2014**, 90,	3.3	28
214	Theory of suppressing avalanche process of carrier in short pulse laser irradiated dielectrics. *Journal of Applied Physics*, **2014**, 115, 203112	2.5	3
213	Ab initio calculations of mechanical properties in □MH2□Hex (M = Er, Sc). *European Physical Journal B*, **2014**, 87, 1	1.2	2
212	Energetics of defects on graphene through fluorination. *ChemSusChem*, **2014**, 7, 1295-300	8.3	9
211	Precipitates of Cr at Σ {112} GB in □Fe. *Materials Research Society Symposia Proceedings*, **2014**, 1645, 1		
210	Cu Segregation at Σ5 Symmetrical Grain Boundary in □Fe: Atomic-Level Simulations. *Chinese Physics Letters*, **2014**, 31, 096801	1.8	3
209	Radiation response of inorganic scintillators: insights from Monte Carlo simulations **2014**,		3
208	Modeling radiation damage near grain boundary in helium-doped □ron. *Nuclear Instruments & Methods in Physics Research B*, **2014**, 332, 426-431	1.2	9
207	First principles prediction of nitrogen-doped carbon nanotubes as a high-performance cathode for Li□ batteries. *RSC Advances*, **2013**, 3, 16775	3.7	40
206	Transition Metal Adsorption Promotes Patterning and Doping of Graphene by Electron Irradiation. *Journal of Physical Chemistry C*, **2013**, 117, 17644-17649	3.8	7
205	Three-dimensional metal-intercalated covalent organic frameworks for near-ambient energy storage. *Scientific Reports*, **2013**, 3, 1882	4.9	28
204	Mechanical and electronic properties of A1□BxHy (A and B = Ti, Zr, Hf) hydride alloys: A first-principles study. *Journal of Alloys and Compounds*, **2013**, 581, 404-412	5.7	5
203	Electron-rich driven electrochemical solid-state amorphization in Li-Si alloys. *Nano Letters*, **2013**, 13, 4511-6	11.5	45
202	Role of cation choice in the radiation tolerance of pyrochlores. *RSC Advances*, **2013**, 3, 2901	3.7	18
201	Excited state electronic properties of sodium iodide and cesium iodide. *Journal of Luminescence*, **2013**, 137, 121-131	3.8	10
200	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, 908-11	11.5	29
199	Ab initio study of He point defects in fcc Au□Ag alloys. *Journal of Alloys and Compounds*, **2013**, 557, 5-10	5.7	4
198	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	1.2	37

197	Diffusion of small He clusters in bulk and grain boundaries in □Fe. *Journal of Nuclear Materials*, **2013**, 442, S667-S673	3.3	29
196	Atomistic studies of nucleation of He clusters and bubbles in bcc iron. *Nuclear Instruments & Methods in Physics Research B*, **2013**, 303, 68-71	1.2	36
195	Formation, stability, and mobility of self-trapped excitations in NaI and NaI1□xTlx from first principles. *Physical Review B*, **2013**, 87,	3.3	17
194	Kinetic Monte Carlo simulations of excitation density dependent scintillation in CsI and CsI(Tl). *Physica Status Solidi (B): Basic Research*, **2013**, 250, 1532-1540	1.3	25
193	In situ nitrogen-doped graphene grown from polydimethylsiloxane by plasma enhanced chemical vapor deposition. *Nanoscale*, **2013**, 5, 600-5	7.7	98
192	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	5.3	28
191	Suppression of nonradiative recombination in ionic insulators by defects: Role of fast electron trapping in Tl-doped CsI. *Physical Review B*, **2013**, 87,	3.3	11
190	Controlling Adsorption Structure of Eosin Y Dye on Nanocrystalline TiO2 Films for Improved Photovoltaic Performances. *Journal of Physical Chemistry C*, **2013**, 117, 14659-14666	3.8	40
189	Effects of temperature on the interactions of helium□vacancy clusters with gliding edge dislocations in □Fe. *Journal of Nuclear Materials*, **2013**, 441, 6-14	3.3	18
188	Electronic structures and magnetic properties of MoS2 nanostructures: atomic defects, nanoholes, nanodots and antidots. *Physical Chemistry Chemical Physics*, **2013**, 15, 10385-94	3.6	98
187	Molecular dynamics simulations of irradiation cascades in alpha-zirconium under macroscopic strain. *Nuclear Instruments & Methods in Physics Research B*, **2013**, 303, 95-99	1.2	32
186	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	8.9	23
185	Electronic origin for the phase transition from amorphous Li(x)Si to crystalline Li15Si4. *ACS Nano*, **2013**, 7, 6303-9	16.7	117
184	Thermal transport properties of rolled graphene nanoribbons. *Applied Physics Letters*, **2013**, 103, 071908	3.4	10
183	Monte Carlo simulation of gamma-ray response of BaF2 and CaF2. *Journal of Applied Physics*, **2013**, 114, 173512	2.5	15
182	Ab initio study of helium behavior in titanium tritides. *Computational Materials Science*, **2013**, 69, 107-113	3.2	16
181	Experimental and computational results on exciton/free-carrier ratio, hot/thermalized carrier diffusion, and linear/nonlinear rate constants affecting scintillator proportionality **2013**,		7
180	Integrated Material System Modeling of Fusion Blanket. *Materials Transactions*, **2013**, 54, 477-483	1.3	1

179	Generalized framework for interatomic potential design: Application to Fe□e system. *Journal of Nuclear Materials*, **2012**, 425, 22-32	3.3	19
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