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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	Lewis acid-base interactions between polysulfides and metal organic framework in lithium sulfur batteries. <i>Nano Letters</i> , 2014 , 14, 2345-52	11.5	529
357	Enhancing radiation tolerance by controlling defect mobility and migration pathways in multicomponent single-phase alloys. <i>Nature Communications</i> , 2016 , 7, 13564	17.4	336
356	The primary damage state in fcc, bcc and hcp metals as seen in molecular dynamics simulations. <i>Journal of Nuclear Materials</i> , 2000 , 276, 1-12	3.3	291
355	Tensile strain switched ferromagnetism in layered NbS ₂ and NbSe ₂ . <i>ACS Nano</i> , 2012 , 6, 9727-36	16.7	265
354	Probing grain boundary sink strength at the nanoscale: Energetics and length scales of vacancy and interstitial absorption by grain boundaries in α -Fe. <i>Physical Review B</i> , 2012 , 85,	3.3	226
353	In situ TEM investigation of congruent phase transition and structural evolution of nanostructured silicon/carbon anode for lithium ion batteries. <i>Nano Letters</i> , 2012 , 12, 1624-32	11.5	222
352	Evolution of lattice structure and chemical composition of the surface reconstruction layer in Li(1.2)Ni(0.2)Mn(0.6)O ₂ cathode material for lithium ion batteries. <i>Nano Letters</i> , 2015 , 15, 514-22	11.5	213
351	Conflicting roles of nickel in controlling cathode performance in lithium ion batteries. <i>Nano Letters</i> , 2012 , 12, 5186-91	11.5	199
350	Atomic scale simulation of defect production in irradiated 3C-SiC. <i>Journal of Applied Physics</i> , 2001 , 90, 2303-2309	2.5	196
349	Computer simulation of defect production by displacement cascades in metals. <i>Nuclear Instruments & Methods in Physics Research B</i> , 1995 , 102, 37-46	1.2	167
348	Analytic modified embedded atom potentials for HCP metals. <i>Journal of Physics Condensed Matter</i> , 2001 , 13, 1193-1213	1.8	142
347	Point-defect and threshold displacement energies in Ni ₃ Al I. Point-defect properties. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 1993 , 67, 275-288		134
346	Radiation-induced segregation on defect clusters in single-phase concentrated solid-solution alloys. <i>Acta Materialia</i> , 2017 , 127, 98-107	8.4	128
345	Properties of helium defects in bcc and fcc metals investigated with density functional theory. <i>Physical Review B</i> , 2009 , 80,	3.3	123
344	A molecular dynamics study of temperature effects on defect production by displacement cascades in α -Fe. <i>Journal of Nuclear Materials</i> , 1997 , 249, 77-86	3.3	121
343	Cascade overlap and amorphization in 3C-SiC: Defect accumulation, topological features, and disordering. <i>Physical Review B</i> , 2002 , 66,	3.3	120
342	Electronic origin for the phase transition from amorphous Li(x)Si to crystalline Li ₁₅ Si ₄ . <i>ACS Nano</i> , 2013 , 7, 6303-9	16.7	117

341	Signal variance in gamma-ray detectorsA review. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2006 , 565, 637-649 ^{1,2}	115
340	Defect production due to displacement cascades in metals as revealed by computer simulation. <i>Journal of Nuclear Materials</i> , 1997 , 251, 1-12	3.3 108
339	Probing the Degradation Mechanism of Li2MnO3 Cathode for Li-Ion Batteries. <i>Chemistry of Materials</i> , 2015 , 27, 975-982	9.6 107
338	Grain growth and phase stability of nanocrystalline cubic zirconia under ion irradiation. <i>Physical Review B</i> , 2010 , 82,	3.3 101
337	Atomic-scale simulation of 50 keV Si displacement cascades in β -SiC. <i>Physical Review B</i> , 2000 , 63,	3.3 101
336	Atomistic study of intrinsic defect migration in 3C-SiC. <i>Physical Review B</i> , 2004 , 69,	3.3 99
335	In situ nitrogen-doped graphene grown from polydimethylsiloxane by plasma enhanced chemical vapor deposition. <i>Nanoscale</i> , 2013 , 5, 600-5	7.7 98
334	Electronic structures and magnetic properties of MoS2 nanostructures: atomic defects, nanoholes, nanodots and antidots. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 10385-94	3.6 98
333	Defect production, multiple ionSolid interactions and amorphization in SiC. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2002 , 191, 487-496	1.2 98
332	Ab initio and empirical-potential studies of defect properties in 3C β -SiC. <i>Physical Review B</i> , 2001 , 64,	3.3 89
331	Modified analytical interatomic potential for a W β system with defects. <i>Journal of Nuclear Materials</i> , 2011 , 408, 12-17	3.3 87
330	Adsorption of hydrogen on boron-doped graphene: A first-principles prediction. <i>Journal of Applied Physics</i> , 2009 , 105, 014309	2.5 86
329	A molecular dynamics study of high-energy displacement cascades in β -Zirconium. <i>Journal of Nuclear Materials</i> , 1998 , 254, 191-204	3.3 86
328	Recovery of close Frenkel pairs produced by low energy recoils in SiC. <i>Journal of Applied Physics</i> , 2003 , 94, 4348-4356	2.5 85
327	A germanium hole spin qubit. <i>Nature Communications</i> , 2018 , 9, 3902	17.4 84
326	Diffusion of He interstitials in grain boundaries in β -Fe. <i>Journal of Nuclear Materials</i> , 2006 , 351, 133-140	3.3 79
325	A new Fe β Fe interatomic potential based on ab initio calculations in β -Fe. <i>Journal of Nuclear Materials</i> , 2011 , 418, 115-120	3.3 75
324	Temperature-dependence of defect creation and clustering by displacement cascades in β -Zirconium. <i>Journal of Nuclear Materials</i> , 2001 , 294, 288-298	3.3 74

323	Shockwave generates dislocation loops in bcc iron. <i>Nature Communications</i> , 2018 , 9, 4880	17.4	74
322	Analytical WBI and HBI interatomic potentials for a WBI system. <i>Journal of Nuclear Materials</i> , 2012 , 426, 31-37	3.3	71
321	Threshold displacement energy in GaN: Ab initio molecular dynamics study. <i>Journal of Applied Physics</i> , 2009 , 105, 123527	2.5	70
320	Atomistic Conversion Reaction Mechanism of WO3 in Secondary Ion Batteries of Li, Na, and Ca. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 6244-7	16.4	70
319	Molecular dynamics study of displacement cascades in Ni3Al I. General features and defect production efficiency. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 1995 , 71, 43-64		69
318	Empirical potential approach for defect properties in 3C-SiC. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2002 , 191, 504-508	1.2	67
317	Defect-enhanced charge transfer by ion-solid interactions in SiC using large-scale ab initio molecular dynamics simulations. <i>Physical Review Letters</i> , 2009 , 103, 027405	7.4	66
316	Formation of stacking-fault tetrahedra in collision cascades. <i>Applied Physics Letters</i> , 1999 , 74, 2720-2722	3.4	64
315	Interaction of helium atoms with edge dislocations in Fe. <i>Journal of Nuclear Materials</i> , 2006 , 351, 141-148	4.3	63
314	Computer simulation of disordering and amorphization by Si and Au recoils in 3C-SiC. <i>Journal of Applied Physics</i> , 2001 , 89, 4275-4281	2.5	61
313	Evidencing the existence of exciting half-metallicity in two-dimensional TiCl3 and VCl3 sheets. <i>Scientific Reports</i> , 2016 , 6, 19407	4.9	60
312	Reaction heterogeneity in practical high-energy lithium-sulfur pouch cells. <i>Energy and Environmental Science</i> , 2020 , 13, 3620-3632	35.4	59
311	Energetic driving force for preferential binding of self-interstitial atoms to Fe grain boundaries over vacancies. <i>Scripta Materialia</i> , 2011 , 64, 908-911	5.6	58
310	Properties and evolution of sessile interstitial clusters produced by displacement cascades in Fe. <i>Journal of Nuclear Materials</i> , 2000 , 276, 213-220	3.3	58
309	Adsorption-induced magnetic properties and metallic behavior of graphene. <i>Applied Physics Letters</i> , 2009 , 95, 123119	3.4	57
308	Modification of Defect Structures in Graphene by Electron Irradiation: Ab Initio Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 16070-16079	3.8	55
307	Electronic and magnetic properties of metal-doped BN sheet: A first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 7588-92	3.6	55
306	Atomistic simulations of the mechanical properties of silicon carbide nanowires. <i>Physical Review B</i> , 2008 , 77,	3.3	54

305	Phase-field modeling of void migration and growth kinetics in materials under irradiation and temperature field. <i>Journal of Nuclear Materials</i> , 2010 , 407, 119-125	3.3	51
304	Point-defect and threshold displacement energies in Ni3Al II. Events at the displacement threshold. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 1993 , 67, 289-306		51
303	The effects of electron-phonon coupling on defect production by displacement cascades in -iron. <i>Modelling and Simulation in Materials Science and Engineering</i> , 1998 , 6, 543-556	2	48
302	Dopant Segregation Boosting High-Voltage Cyclability of Layered Cathode for Sodium Ion Batteries. <i>Advanced Materials</i> , 2019 , 31, e1904816	24	46
301	Molecular dynamics simulation of helium cluster diffusion and bubble formation in bulk tungsten. <i>Journal of Nuclear Materials</i> , 2014 , 455, 544-548	3.3	46
300	Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage. <i>Acta Materialia</i> , 2020 , 196, 133-143	8.4	45
299	Electron-rich driven electrochemical solid-state amorphization in Li-Si alloys. <i>Nano Letters</i> , 2013 , 13, 4511-4516	11.65	45
298	Threshold displacement energies and defect formation energies in Y2Ti2O7. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 415801	1.8	44
297	Ab initio investigation of phase stability of Y2Ti2O7 and Y2Zr2O7 under high pressure. <i>Physical Review B</i> , 2009 , 80,	3.3	44
296	Molecular-confinement of polysulfides within mesoscale electrodes for the practical application of lithium sulfur batteries. <i>Nano Energy</i> , 2015 , 13, 267-274	17.1	43
295	Computer simulation of electron thermalization in CsI and CsI(Tl). <i>Journal of Applied Physics</i> , 2011 , 110, 064903	2.5	43
294	Atomic-scale simulation of displacement cascades and amorphization in SiC. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2001 , 180, 176-186	1.2	42
293	Electronic and magnetic properties of substituted BN sheets: a density functional theory study. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7378-83	3.6	41
292	Atomistic simulation of helium-defect interaction in alpha-iron. <i>Applied Physics Letters</i> , 2006 , 88, 091915	3.4	41
291	Native defect properties in SiC: Ab initio and empirical potential calculations. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2001 , 180, 286-292	1.2	41
290	First principles prediction of nitrogen-doped carbon nanotubes as a high-performance cathode for LiB batteries. <i>RSC Advances</i> , 2013 , 3, 16775	3.7	40
289	Controlling Adsorption Structure of Eosin Y Dye on Nanocrystalline TiO2 Films for Improved Photovoltaic Performances. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 14659-14666	3.8	40
288	Computer simulation of the light yield nonlinearity of inorganic scintillators. <i>Journal of Applied Physics</i> , 2009 , 105, 114915	2.5	40

287	First-principles study of electronic properties of La ₂ Hf ₂ O ₇ and Gd ₂ Hf ₂ O ₇ . <i>Journal of Applied Physics</i> , 2007 , 102, 063704	2.5	40
286	Intrinsic defect properties in GaN calculated by ab initio and empirical potential methods. <i>Physical Review B</i> , 2004 , 70,	3.3	40
285	Zirconate pyrochlores under high pressure. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 12472-7	3.6	39
284	Atomistic simulations of the size, orientation, and temperature dependence of tensile behavior in GaN nanowires. <i>Physical Review B</i> , 2007 , 76,	3.3	39
283	Computer simulation of displacement cascade effects in metals. <i>Radiation Effects and Defects in Solids</i> , 1997 , 141, 283-310	0.9	38
282	Atomistic simulation of the size and orientation dependences of thermal conductivity in GaN nanowires. <i>Applied Physics Letters</i> , 2007 , 90, 161923	3.4	38
281	Phase-field simulations of intragranular fission gas bubble evolution in UO ₂ under post-irradiation thermal annealing. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2013 , 303, 62-67	1.2	37
280	Mechanical properties and elastic constants due to damage accumulation and amorphization in SiC. <i>Physical Review B</i> , 2004 , 69,	3.3	37
279	Atomistic study of the migration of di- and tri-interstitials in silicon. <i>Physical Review B</i> , 2005 , 71,	3.3	37
278	Atomistic studies of nucleation of He clusters and bubbles in bcc iron. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2013 , 303, 68-71	1.2	36
277	Energy dissipation and defect generation in nanocrystalline silicon carbide. <i>Physical Review B</i> , 2010 , 81,	3.3	36
276	Atomistic modeling of helium interacting with screw dislocations in Fe. <i>Journal of Nuclear Materials</i> , 2007 , 367-370, 311-315	3.3	36
275	Effects of local structure on helium bubble growth in bulk and at grain boundaries of bcc iron: A molecular dynamics study. <i>Acta Materialia</i> , 2015 , 97, 86-93	8.4	35
274	New interatomic potentials of W, Re and W-Re alloy for radiation defects. <i>Journal of Nuclear Materials</i> , 2018 , 502, 141-153	3.3	35
273	Structural and bonding properties of stannate pyrochlores: A density functional theory investigation. <i>Computational Materials Science</i> , 2008 , 42, 653-658	3.2	35
272	Novel Electronic and Magnetic Properties of Graphene Nanoflakes in a Boron Nitride Layer. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 7581-7586	3.8	34
271	Monte Carlo simulations of defect recovery within a 10 keV collision cascade in 3C2SiC. <i>Journal of Applied Physics</i> , 2007 , 102, 103508	2.5	34
270	Atomistic simulations of helium clustering and grain boundary reconstruction in alpha-iron. <i>Acta Materialia</i> , 2015 , 82, 275-286	8.4	33

269	Understanding the presence of vacancy clusters in ZnO from a kinetic perspective. <i>Applied Physics Letters</i> , 2014 , 104, 252101	3.4	33
268	Electronic and optical properties of two-dimensional covalent organic frameworks. <i>Journal of Materials Chemistry</i> , 2012 , 22, 16964		33
267	First principles study of electronic properties of gallium nitride nanowires grown along different crystal directions. <i>Computational Materials Science</i> , 2010 , 50, 344-348	3.2	33
266	Migration of vacancies, He interstitials and He-vacancy clusters at grain boundaries in δ Fe. <i>Journal of Nuclear Materials</i> , 2009 , 386-388, 390-394	3.3	33
265	First-principles calculation of structural and energetic properties for $A_2Ti_2O_7$ (A = Lu, Er, Y, Gd, Sm, Nd, La). <i>Journal of Materials Research</i> , 2009 , 24, 1335-1341	2.5	33
264	Amorphization of silicon carbide by carbon displacement. <i>Applied Physics Letters</i> , 2004 , 84, 3909-3911	3.4	33
263	Molecular dynamics simulations of irradiation cascades in alpha-zirconium under macroscopic strain. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2013 , 303, 95-99	1.2	32
262	Tensile and compressive mechanical behavior of twinned silicon carbide nanowires. <i>Acta Materialia</i> , 2010 , 58, 1963-1971	8.4	32
261	Diffusion of He interstitial and di-He cluster at grain boundaries in δ Fe. <i>Journal of Nuclear Materials</i> , 2007 , 367-370, 446-450	3.3	32
260	Damage accumulation and defect relaxation in 4H β SiC. <i>Physical Review B</i> , 2004 , 70,	3.3	32
259	The effects of interfaces on radiation damage production in layered metal composites. <i>Journal of Nuclear Materials</i> , 2004 , 329-333, 924-928	3.3	32
258	First-principles calculations of pressure-induced phase transformation in AlN and GaN. <i>Computational Materials Science</i> , 2010 , 48, 768-772	3.2	31
257	Molecular dynamics modeling of the thermal conductivity of irradiated SiC as a function of cascade overlap. <i>Journal of Applied Physics</i> , 2007 , 101, 023527	2.5	31
256	The influence of strain on defect generation by displacement cascades in δ iron. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2001 , 180, 187-193	1.2	31
255	Study of loop-loop and loop-edge dislocation interactions in bcc iron. <i>Journal of Nuclear Materials</i> , 2000 , 283-287, 784-788	3.3	31
254	Regulating energy transfer of excited carriers and the case for excitation-induced hydrogen dissociation on hydrogenated graphene. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 908-11	11.5	29
253	Diffusion of small He clusters in bulk and grain boundaries in δ Fe. <i>Journal of Nuclear Materials</i> , 2013 , 442, S667-S673	3.3	29
252	Monte Carlo simulations of electron thermalization in alkali iodide and alkaline-earth fluoride scintillators. <i>Journal of Applied Physics</i> , 2012 , 112, 014906	2.5	29

251	Modeling of He-defect interactions in ferritic alloys for fusion. <i>Journal of Nuclear Materials</i> , 2008 , 382, 134-142	3.3	29
250	Primary damage states produced by Si and Au recoils in SiC: A molecular dynamics and experimental investigation. <i>Physical Review B</i> , 2001 , 63,	3.3	29
249	Molecular dynamics study of displacement cascades in Ni3Al II. Kinetics, disordering and atomic mixing. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 1995 , 71, 65-84		29
248	Three-dimensional metal-intercalated covalent organic frameworks for near-ambient energy storage. <i>Scientific Reports</i> , 2013 , 3, 1882	4.9	28
247	Interplay between atomic disorder, lattice swelling, and defect energy in ion-irradiation-induced amorphization of SiC. <i>Physical Review B</i> , 2014 , 90,	3.3	28
246	Blunting of a brittle crack at grain boundaries: An atomistic study in BCC Iron. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2013 , 576, 231-238	5.3	28
245	Gamma-ray interaction in Ge: A Monte Carlo simulation. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 255, 286-290	1.2	28
244	Ab initio study of formation, migration and binding properties of helium-vacancy clusters in aluminum. <i>Physica B: Condensed Matter</i> , 2008 , 403, 2719-2724	2.8	28
243	Atomic-level study of melting behavior of GaN nanotubes. <i>Journal of Applied Physics</i> , 2006 , 100, 063503	2.5	28
242	Enhanced Radiation-tolerant Oxide Dispersion Strengthened Steel and its Microstructure Evolution under Helium-implantation and Heavy-ion Irradiation. <i>Scientific Reports</i> , 2017 , 7, 40343	4.9	27
241	Enhanced void swelling in NiCoFeCrPd high-entropy alloy by indentation-induced dislocations. <i>Materials Research Letters</i> , 2018 , 6, 584-591	7.4	27
240	Binding energetics of substitutional and interstitial helium and di-helium defects with grain boundary structure in α -Fe. <i>Journal of Applied Physics</i> , 2014 , 115, 033503	2.5	26
239	H ⁺ diffusion and electrochemical stability of Li _{1+x+y} Al _x Ti _{2-x} Si _y P _{3-y} O ₁₂ glass in aqueous Li/air battery electrolytes. <i>Journal of Power Sources</i> , 2012 , 214, 292-297	8.9	26
238	Defects in gallium nitride nanowires: First principles calculations. <i>Journal of Applied Physics</i> , 2010 , 108, 044305	2.5	26
237	Atomic-scale modeling of interactions of helium, vacancies and helium-vacancy clusters with screw dislocations in alpha-iron. <i>Philosophical Magazine</i> , 2010 , 90, 885-895	1.6	26
236	Spin and band-gap engineering in copper-doped BN sheet. <i>Chemical Physics Letters</i> , 2010 , 491, 203-207	2.5	26
235	Monte Carlo method for simulating γ -ray interaction with materials: A case study on Si. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2007 , 579, 292-296	1.2	26
234	Kinetic Monte Carlo Annealing Simulation of Damage Produced by Cascades in Alpha-Iron. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 540, 703		26

233	Synthesis of CN dual-doped Cr ₂ O ₃ visible light-driven photocatalysts derived from metalorganic framework (MOF) for cyclohexane oxidation. <i>RSC Advances</i> , 2016 , 6, 84871-84881	3.7	25
232	Kinetic Monte Carlo simulations of excitation density dependent scintillation in CsI and CsI(Tl). <i>Physica Status Solidi (B): Basic Research</i> , 2013 , 250, 1532-1540	1.3	25
231	Dynamic interactions of helium-vacancy clusters with edge dislocations in δ -Fe. <i>Physica B: Condensed Matter</i> , 2010 , 405, 1754-1758	2.8	25
230	Dislocation-accelerated void formation under irradiation in zirconium. <i>Acta Materialia</i> , 2015 , 82, 94-99	8.4	24
229	Coupling a Germanium Hut Wire Hole Quantum Dot to a Superconducting Microwave Resonator. <i>Nano Letters</i> , 2018 , 18, 2091-2097	11.5	24
228	Irradiation-induced defect clustering and amorphization in silicon carbide. <i>Journal of Materials Research</i> , 2010 , 25, 2349-2353	2.5	24
227	Codoping of magnesium with oxygen in gallium nitride nanowires. <i>Applied Physics Letters</i> , 2010 , 96, 103112	3.12	24
226	Interaction of helium-vacancy clusters with edge dislocations in δ -Fe. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 265, 541-546	1.2	24
225	Finding possible transition states of defects in silicon-carbide and alpha-iron using the dimer method. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2003 , 202, 1-7	1.2	24
224	Energetics of vacancy segregation to [100] symmetric tilt grain boundaries in bcc tungsten. <i>Scientific Reports</i> , 2016 , 6, 36955	4.9	23
223	Interplay between two-phase and solid solution reactions in high voltage spinel cathode material for lithium ion batteries. <i>Journal of Power Sources</i> , 2013 , 242, 736-741	8.9	23
222	Ab initio study of intrinsic, H, and He point defects in hcp-Er. <i>Journal of Applied Physics</i> , 2010 , 107, 054903	3.5	23
221	He _n cluster nucleation and growth in δ -Fe grain boundaries. <i>Acta Materialia</i> , 2017 , 124, 544-555	8.4	22
220	Dislocation mechanism of deuterium retention in tungsten under plasma implantation. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 395001	1.8	22
219	Molecular dynamics simulation of interaction of H with vacancy in W. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2009 , 267, 3197-3199	1.2	22
218	First-principles study of energetic and electronic properties of A ₂ Ti ₂ O ₇ (A=Sm, Gd, Er) pyrochlore. <i>Journal of Applied Physics</i> , 2008 , 104, 073503	2.5	22
217	Computer simulations of interstitial loop growth kinetics in irradiated bcc Fe. <i>Journal of Nuclear Materials</i> , 2012 , 427, 259-267	3.3	21
216	Effects of interatomic potential on He bubble creation by cascades in δ -Fe. <i>Journal of Applied Physics</i> , 2008 , 103, 063528	2.5	21

215	Atomic-scale simulations of cascade overlap and damage evolution in silicon carbide. <i>Journal of Materials Research</i> , 2003 , 18, 1877-1883	2.5	21
214	A comparative study of the structure and energetics of elementary defects in 3C- and 4H-SiC. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, 1307-1323	1.8	21
213	Carrier-Multiplication-Induced Structural Change during Ultrafast Carrier Relaxation and Nonthermal Phase Transition in Semiconductors. <i>Physical Review Letters</i> , 2016 , 117, 126402	7.4	20
212	Interstitial migration behavior and defect evolution in ion irradiated pure nickel and Ni-xFe binary alloys. <i>Journal of Nuclear Materials</i> , 2018 , 509, 237-244	3.3	20
211	Yield, variance and spatial distribution of electron-hole pairs in CsI. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2011 , 652, 564-567	1.2	20
210	Controlling electronic structures by irradiation in single-walled SiC nanotubes: a first-principles molecular dynamics study. <i>Nanotechnology</i> , 2009 , 20, 075708	3.4	20
209	First-principles study of the noble metal-doped BN layer. <i>Journal of Applied Physics</i> , 2011 , 109, 084308	2.5	20
208	First-principles calculation of defect formation energies and electronic properties in stannate pyrochlores. <i>Journal of Applied Physics</i> , 2008 , 104, 093702	2.5	20
207	Generalized framework for interatomic potential design: Application to Fe-H system. <i>Journal of Nuclear Materials</i> , 2012 , 425, 22-32	3.3	19
206	Hydrogenated Graphene Nanoflakes: Semiconductor to Half-Metal Transition and Remarkable Large Magnetism. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 5531-5537	3.8	19
205	Atomic-scale computer simulation of primary irradiation damage effects in metals. <i>Journal of Computer-Aided Materials Design</i> , 1999 , 6, 225-237		19
204	Revealing reaction mechanisms of nanoconfined LiS: implications for lithium-sulfur batteries. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 11713-11721	3.6	18
203	Role of cation choice in the radiation tolerance of pyrochlores. <i>RSC Advances</i> , 2013 , 3, 2901	3.7	18
202	Effects of temperature on the interactions of helium-vacancy clusters with gliding edge dislocations in Fe. <i>Journal of Nuclear Materials</i> , 2013 , 441, 6-14	3.3	18
201	First-principles study of the electronic properties of wurtzite, zinc-blende, and twinned InP nanowires. <i>Nanotechnology</i> , 2010 , 21, 505709	3.4	18
200	Defect production and formation of helium-vacancy clusters due to cascades in Fe. <i>Physica B: Condensed Matter</i> , 2007 , 391, 179-185	2.8	18
199	Molecular dynamics simulation of the structural, elastic, and thermal properties of pyrochlores. <i>RSC Advances</i> , 2016 , 6, 41410-41419	3.7	18
198	Self-healing mechanism of irradiation defects in nickel-graphene nanocomposite: An energetic and kinetic perspective. <i>Journal of Alloys and Compounds</i> , 2018 , 765, 253-263	5.7	18

197	Formation, stability, and mobility of self-trapped excitations in NaI and NaI δ Tlx from first principles. <i>Physical Review B</i> , 2013 , 87,	3.3	17
196	Ab initio study of stability and migration of point defects in copper-graphene layered composite. <i>Journal of Alloys and Compounds</i> , 2017 , 692, 49-58	5.7	17
195	Diffusion of tungsten clusters on tungsten (110) surface. <i>European Physical Journal B</i> , 2009 , 68, 479-485	1.2	17
194	Structural phase transitions in high-pressure wurtzite to rocksalt phase in GaN and SiC. <i>Applied Physics Letters</i> , 2008 , 92, 241909	3.4	17
193	The effect of Mo addition on structure and glass forming ability of Ni-Zr alloys. <i>Journal of Alloys and Compounds</i> , 2019 , 775, 1184-1198	5.7	17
192	Measuring hole spin states of single quantum dot in germanium hut wire. <i>Applied Physics Letters</i> , 2017 , 110, 133105	3.4	16
191	The interactions between rhenium and interstitial-type defects in bulk tungsten: A combined study by molecular dynamics and molecular statics simulations. <i>Journal of Nuclear Materials</i> , 2019 , 522, 200-213	3.3	16
190	Ab initio study of helium behavior in titanium tritides. <i>Computational Materials Science</i> , 2013 , 69, 107-113	1.2	16
189	Ab initio molecular dynamics simulations of low energy recoil events in ceramics. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2011 , 269, 1693-1697	1.2	16
188	Defect production by near-surface displacement cascades in Ni ₃ Al. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 1997 , 75, 1603-1623		16
187	. <i>IEEE Transactions on Nuclear Science</i> , 2008 , 55, 1079-1085	1.7	16
186	A first-principles investigation of the ScO ₂ monolayer as the cathode material for alkali metal-ion batteries. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 3171-3180	1.3	15
185	Binding of HenV clusters to Fe grain boundaries. <i>Journal of Applied Physics</i> , 2014 , 115, 233501	2.5	15
184	Monte Carlo simulation of gamma-ray response of BaF ₂ and CaF ₂ . <i>Journal of Applied Physics</i> , 2013 , 114, 173512	2.5	15
183	Stone-Wales defects created by low energy recoils in single-walled silicon carbide nanotubes. <i>Journal of Applied Physics</i> , 2009 , 106, 084305	2.5	15
182	Substrate-induced magnetism in BN layer: A first-principles study. <i>Solid State Communications</i> , 2011 , 151, 883-886	1.6	15
181	A first-principles study of the structural, mechanical and electronic properties of precipitates of AlCu in Al-Cu alloys. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 967-976	3.6	15
180	Site-Controlled Uniform Ge/Si Hut Wires with Electrically Tunable Spin-Orbit Coupling. <i>Advanced Materials</i> , 2020 , 32, e1906523	2.4	14

179	Displacement damage and predicted non-ionizing energy loss in GaAs. <i>Journal of Applied Physics</i> , 2017 , 121, 095104	2.5	13
178	New interatomic potentials for studying the behavior of noble gas atoms in tungsten. <i>Journal of Nuclear Materials</i> , 2015 , 467, 398-405	3.3	13
177	Atomistic Conversion Reaction Mechanism of WO ₃ in Secondary Ion Batteries of Li, Na, and Ca. <i>Angewandte Chemie</i> , 2016 , 128, 6352-6355	3.6	13
176	Embedded-atom method potential for modeling hydrogen and hydrogen-defect interaction in tungsten. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 435401	1.8	13
175	Structure and Electronic Properties of Saturated and Unsaturated Gallium Nitride Nanotubes. <i>Journal of Physical Chemistry C</i> , 2009 , 113, 19281-19285	3.8	13
174	Electronic and magnetic properties of Al adsorption on Uranium (001) surface: Ab initio calculations. <i>Journal of Alloys and Compounds</i> , 2009 , 476, 675-682	5.7	13
173	Ab initio calculations of structural and energetic properties of defects in gallium nitride. <i>Journal of Applied Physics</i> , 2008 , 103, 123529	2.5	13
172	Molecular dynamics simulations of high-energy radiation damage in W and WRe alloys. <i>Journal of Nuclear Materials</i> , 2019 , 524, 9-20	3.3	12
171	Irradiation effects of medium-entropy alloy NiCoCr with and without pre-indentation. <i>Journal of Nuclear Materials</i> , 2019 , 524, 60-66	3.3	12
170	Interplay between intrinsic point defects and low-angle grain boundary in bcc tungsten: effects of local stress field. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 255007	1.8	12
169	Effects of surface defects on two-dimensional electron gas at NdAlO ₃ /SrTiO ₃ interface. <i>Scientific Reports</i> , 2014 , 4, 5477	4.9	12
168	Monte Carlo simulation of electron thermalization in scintillator materials: Implications for scintillator nonproportionality. <i>Journal of Applied Physics</i> , 2017 , 122, 234504	2.5	12
167	Electronic and magnetic properties of C-adsorbed graphene: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 16574-8	3.6	12
166	Stability of helium clusters during displacement cascades. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 255, 63-67	1.2	12
165	Computational simulation of threshold displacement energies of GaAs. <i>Journal of Materials Research</i> , 2017 , 32, 1555-1562	2.5	11
164	"H ₂ sponge": pressure as a means for reversible high-capacity hydrogen storage in nanoporous Ca-intercalated covalent organic frameworks. <i>Nanoscale</i> , 2015 , 7, 6319-24	7.7	11
163	Nucleation of Cr precipitates in FeCr alloy under irradiation. <i>Computational Materials Science</i> , 2015 , 101, 293-300	3.2	11
162	Pressure effect on stabilities of self-interstitials in HCP-zirconium. <i>Scientific Reports</i> , 2014 , 4, 5735	4.9	11

161	New understanding of nano-scale interstitial dislocation loops in BCC iron. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 455301	1.8	11
160	Suppression of nonradiative recombination in ionic insulators by defects: Role of fast electron trapping in Tl-doped CsI. <i>Physical Review B</i> , 2013 , 87,	3.3	11
159	Application of the phase-field method in predicting gas bubble microstructure evolution in nuclear fuels. <i>International Journal of Materials Research</i> , 2010 , 101, 515-522	0.5	11
158	Helium nanobubble release from Pd surface: An atomic simulation. <i>Journal of Materials Research</i> , 2011 , 26, 416-423	2.5	11
157	Size dependence of melting of GaN nanowires with triangular cross sections. <i>Journal of Applied Physics</i> , 2007 , 101, 043511	2.5	11
156	Temperature effects on defect production and disordering by displacement cascades in Ni ₃ Al. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 2000 , 80, 1453-1468		11
155	Shear-coupled grain boundary migration assisted by unusual atomic shuffling. <i>Scientific Reports</i> , 2016 , 6, 23602	4.9	11
154	Development of the interatomic potentials for W-Ta system. <i>Computational Materials Science</i> , 2019 , 163, 91-99	3.2	10
153	Atomistic insights into shear-coupled grain boundary migration in bcc tungsten. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2016 , 677, 20-28	5.3	10
152	Atomistic study of hydrogen behavior around dislocations in Fe. <i>Journal of Nuclear Materials</i> , 2018 , 510, 219-228	3.3	10
151	Kinetic Monte Carlo Simulations of Scintillation Processes in NaI(Tl). <i>IEEE Transactions on Nuclear Science</i> , 2014 , 61, 860-869	1.7	10
150	Excited state electronic properties of sodium iodide and cesium iodide. <i>Journal of Luminescence</i> , 2013 , 137, 121-131	3.8	10
149	Grain boundary resistance to amorphization of nanocrystalline silicon carbide. <i>Scientific Reports</i> , 2015 , 5, 16602	4.9	10
148	Thermal transport properties of rolled graphene nanoribbons. <i>Applied Physics Letters</i> , 2013 , 103, 071908	3.4	10
147	Functionalized graphene nanoroads for quantum well device. <i>Applied Physics Letters</i> , 2011 , 98, 093108	3.4	10
146	Multiple-interactions of displacement cascades with He-vacancy clusters in Fe: Computer simulations. <i>Journal of Nuclear Materials</i> , 2008 , 374, 437-444	3.3	10
145	Mobility of Self-Interstitials in FCC and BCC Metals. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 527, 49		10
144	Crossover from disordered to core-shell structures of nano-oxide Y ₂ O ₃ dispersed particles in Fe. <i>Applied Physics Letters</i> , 2016 , 109, 031911	3.4	10

143	Proton irradiation of graphene: insights from atomistic modeling. <i>Nanoscale</i> , 2019 , 11, 20754-20765	7.7	10
142	Mechanisms for interstitial dislocation loops to diffuse in BCC iron. <i>Nature Communications</i> , 2021 , 12, 225	17.4	10
141	Ab initio study of interstitial helium clusters in 3C-SiC. <i>Journal of Nuclear Materials</i> , 2019 , 521, 13-20	3.3	9
140	Effect of hydrogen on grain boundary migration in tungsten. <i>Science China: Physics, Mechanics and Astronomy</i> , 2015 , 58, 1-9	3.6	9
139	Calculation of energy relaxation rates of fast particles by phonons in crystals. <i>Physical Review B</i> , 2015 , 91,	3.3	9
138	Atomic-Scale Simulation for Pseudometallic Defect-Generation Kinetics and Effective NIEL in GaN. <i>IEEE Transactions on Nuclear Science</i> , 2018 , 65, 1108-1118	1.7	9
137	First-principles search for efficient activators for LaI3. <i>Journal of Luminescence</i> , 2016 , 176, 227-234	3.8	9
136	Energetics and structures of hydrogen-vacancy clusters in tungsten based on genetic algorithm. <i>Science China: Physics, Mechanics and Astronomy</i> , 2018 , 61, 1	3.6	9
135	Energetics of defects on graphene through fluorination. <i>ChemSusChem</i> , 2014 , 7, 1295-300	8.3	9
134	Modeling radiation damage near grain boundary in helium-doped Fe. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2014 , 332, 426-431	1.2	9
133	Ab initio study of defect properties in YPO4. <i>Computational Materials Science</i> , 2012 , 54, 170-175	3.2	9
132	Band-Gap Engineering of Carbon Nanotubes with Grain Boundaries. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 2271-2277	3.8	9
131	Evolution kinetics of interstitial loops in irradiated materials: a phase-field model. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2012 , 20, 015011	2	9
130	Mechanical behavior of twinned SiC nanowires under combined tension-torsion and compression-torsion strain. <i>Journal of Applied Physics</i> , 2010 , 108, 013504	2.5	9
129	Theory of absorption rate of carriers in fused silica under intense laser irradiation. <i>Journal of Applied Physics</i> , 2010 , 108, 103116	2.5	9
128	Effect of vacancy on the sliding of an iron grain boundary. <i>Journal of Applied Physics</i> , 2011 , 109, 113512	2.5	9
127	Atomic-level simulations of epitaxial recrystallization and amorphous-to-crystalline transition in 4H-SiC. <i>Physical Review B</i> , 2006 , 74,	3.3	9
126	Atomic-scale simulations of multiple ion-solid interactions and structural evolution in silicon carbide. <i>Journal of Materials Research</i> , 2002 , 17, 259-262	2.5	9

125	Spontaneous ripple formation in phosphorene: electronic properties and possible applications. <i>Nanoscale</i> , 2016 , 8, 11827-33	7.7	9
124	Effects of interstitial defects on stress-driven grain boundary migration in bcc tungsten. <i>Journal of Nuclear Materials</i> , 2018 , 512, 246-251	3.3	9
123	Long-time atomistic dynamics through a new self-adaptive accelerated molecular dynamics method. <i>Journal of Physics Condensed Matter</i> , 2017 , 29, 145201	1.8	8
122	Evolution of nanoscale interstitial dislocation loops under coupling effect of stress and temperature. <i>Scripta Materialia</i> , 2017 , 136, 64-67	5.6	8
121	Evolution of vacancy defects in heavy ion irradiated tungsten exposed to helium plasma. <i>Journal of Nuclear Materials</i> , 2020 , 532, 152051	3.3	8
120	Structural evolution of NiAu nanoparticles under ambient conditions directly revealed by atom-resolved imaging combined with DFT simulation. <i>Nanoscale</i> , 2014 , 6, 12898-904	7.7	8
119	Prediction of thermal conductivity for irradiated SiC/SiC composites by informing continuum models with molecular dynamics data. <i>Journal of Nuclear Materials</i> , 2014 , 448, 364-372	3.3	8
118	Ab initio study of stability and migration of H and He in hcp-Sc. <i>Journal of Physics Condensed Matter</i> , 2011 , 23, 035701	1.8	8
117	Bond-Order Potential for Erbium-Hydride System. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 25097-25104	3.8	8
116	Phase-field modeling of void evolution and swelling in materials under irradiation. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011 , 54, 856-865	3.6	8
115	Ab initio molecular dynamics simulation of a pressure induced zinc blende to rocksalt phase transition in SiC. <i>Journal of Physics Condensed Matter</i> , 2009 , 21, 245801	1.8	8
114	Ab initio study of H and He migrations in fphase Sc, Y, and Er hydrides. <i>Chinese Physics B</i> , 2012 , 21, 056601	1.2	8
113	Thermodynamic Calculation of Phase Equilibria in the Sn-Ag-Cu-Ni-Au System. <i>Journal of Electronic Materials</i> , 2007 , 36, 1429-1441	1.9	8
112	First-principles study of sulfur passivation of GaP(001) surfaces at one-monolayer coverage. <i>Solid State Communications</i> , 2008 , 147, 141-145	1.6	8
111	Glissile and Sessile Vacancy and Self-Interstitial Clusters in BCC and FCC Metals. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 540, 691		8
110	. <i>IEEE Transactions on Plasma Science</i> , 2017 , 45, 289-293	1.3	7
109	Understanding the release of helium atoms from nanochannel tungsten: a molecular dynamics simulation. <i>Nuclear Fusion</i> , 2019 , 59, 076020	3.3	7
108	Evidencing the existence of intrinsic half-metallicity and ferromagnetism in zigzag gallium sulfide nanoribbons. <i>Scientific Reports</i> , 2014 , 4, 5773	4.9	7

107	Elucidating He-H assisted cavity evolution in alpha Cr under multiple ion beam irradiation. <i>Scripta Materialia</i> , 2020 , 187, 291-295	5.6	7
106	Atomistic insights into the reaction mechanism of nanostructured LiI: Implications for rechargeable Li-I2 batteries. <i>Energy Storage Materials</i> , 2019 , 17, 211-219	19.4	7
105	Transition Metal Adsorption Promotes Patterning and Doping of Graphene by Electron Irradiation. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 17644-17649	3.8	7
104	High performance computing for advanced modeling and simulation of materials. <i>Computer Physics Communications</i> , 2017 , 211, 1	4.2	7
103	Experimental and computational results on exciton/free-carrier ratio, hot/thermalized carrier diffusion, and linear/nonlinear rate constants affecting scintillator proportionality 2013 ,		7
102	Phase transition in nanocrystalline iron: Atomistic-level simulations. <i>International Journal of Materials Research</i> , 2010 , 101, 1361-1368	0.5	7
101	Ab initio study of the stability of intrinsic and extrinsic Ag point defects in 3CSiC. <i>Journal of Nuclear Materials</i> , 2018 , 510, 596-602	3.3	7
100	Perspectives on multiscale modelling and experiments to accelerate materials development for fusion. <i>Journal of Nuclear Materials</i> , 2021 , 554, 153113	3.3	7
99	Enhanced formation of and interstitial loops by helium clustering in bcc iron. <i>Materials Letters</i> , 2017 , 190, 260-262	3.3	6
98	An ab initio study for probing iodization reactions on metallic anode surfaces of LiI2 batteries. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 7807-7814	13	6
97	Theoretical prediction of LiScO nanosheets as a cathode material for Li-O batteries. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 22351-22358	3.6	6
96	First-principles study of He point-defects in HCP rare-earth metals. <i>Science China: Physics, Mechanics and Astronomy</i> , 2011 , 54, 827-830	3.6	6
95	Migration of Cr-vacancy clusters and interstitial Cr in Fe using the dimer method. <i>Physical Review B</i> , 2010 , 81,	3.3	6
94	Experimental Investigation and Thermodynamic Assessment of Phase Equilibria in the Ag-Au-Sn System. <i>Journal of Electronic Materials</i> , 2009 , 38, 2096-2105	1.9	6
93	Migration of point defects and a defect pair in zinc oxide using the dimer method. <i>Journal of Materials Research</i> , 2012 , 27, 2241-2248	2.5	6
92	Atomistic study of the melting behavior of single crystalline wurtzite gallium nitride nanowires. <i>Journal of Materials Research</i> , 2007 , 22, 742-747	2.5	6
91	Interatomic potentials and defect properties of Fe-Cr-Al alloys. <i>Journal of Nuclear Materials</i> , 2020 , 541, 152421	3.3	6
90	Unraveling TM Migration Mechanisms in LiNiMnCoO by Modeling and Experimental Studies. <i>Nano Letters</i> , 2021 , 21, 6875-6881	11.5	6

89	Reveal the fast and charge-insensitive lattice diffusion of silver in cubic silicon carbide via first-principles calculations. <i>Computational Materials Science</i> , 2019 , 170, 109190	3.2	5
88	Molecular dynamics simulations of radiation damage generation and dislocation loop evolution in Ni and binary Ni-based alloys. <i>Computational Materials Science</i> , 2020 , 177, 109555	3.2	5
87	Interatomic potentials of W/V and W/Mo binary systems for point defects studies. <i>Journal of Nuclear Materials</i> , 2020 , 531, 152020	3.3	5
86	Mechanical and electronic properties of A _{1-x} B _x H _y (A and B = Ti, Zr, Hf) hydride alloys: A first-principles study. <i>Journal of Alloys and Compounds</i> , 2013 , 581, 404-412	5.7	5
85	Ab initio molecular dynamics simulation of structural transformation in zinc blende GaN under high pressure. <i>Journal of Alloys and Compounds</i> , 2010 , 490, 537-540	5.7	5
84	Charge separation in wurtzite/zinc-blende heterojunction GaN nanowires. <i>ChemPhysChem</i> , 2010 , 11, 3329-32	3.2	5
83	Computer Simulation of Defect Production and Behaviour in Displacement Cascades in Metals. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 540, 617		5
82	Computer Simulation of Displacement Cascade Damage in Metals. <i>Materials Research Society Symposia Proceedings</i> , 1994 , 373, 15		5
81	Ultrafast coherent control of a hole spin qubit in a germanium quantum dot.. <i>Nature Communications</i> , 2022 , 13, 206	17.4	5
80	Anisotropic γ -Factor and Spin-Orbit Field in a Germanium Hut Wire Double Quantum Dot. <i>Nano Letters</i> , 2021 , 21, 3835-3842	11.5	5
79	Development of a Ni/Mo interatomic potential for irradiation simulation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019 , 27, 045009	2	4
78	Zero Field Splitting of Heavy-Hole States in Quantum Dots. <i>Nano Letters</i> , 2020 , 20, 5201-5206	11.5	4
77	Ab initio study of He point defects in fcc Au/Ag alloys. <i>Journal of Alloys and Compounds</i> , 2013 , 557, 5-10	5.7	4
76	Oxygen-induced magnetic properties and metallic behavior of a BN sheet. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 465303	1.8	4
75	Effects of Fe/He potential on primary damage formation in Fe-1%He. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2009 , 267, 3046-3049	1.2	4
74	Production of Very Fine Grained Mg ₈₀ Al ₁₀ Zn Alloy by Continuous Extrusion Forming (CONFORM). <i>Advanced Engineering Materials</i> , 2010 , 12, 843-847	3.5	4
73	Model of plasmon decay for electron cascade simulation. <i>Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment</i> , 2007 , 579, 454-457	1.2	4
72	The Effect of Temperature on Defect Production by Displacement Cascades in α -Fe. <i>Materials Research Society Symposia Proceedings</i> , 1996 , 439, 307		4

71	Atomistic simulations of the interaction between transmutation-produced Re and grain boundaries in tungsten. <i>Computational Materials Science</i> , 2020 , 173, 109412	3.2	4
70	Molecular dynamics simulation of the diffusion of self-interstitial atoms and interstitial loops under temperature gradient field in tungsten. <i>Journal of Applied Physics</i> , 2020 , 128, 065103	2.5	4
69	Study of plasma induced nanostructure formation and surface morphology changes on tungsten and stainless steel at atmospheric pressure. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2019 , 37, 011301	2.9	4
68	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. <i>Journal of Nuclear Materials</i> , 2019 , 526, 151766	3.3	3
67	Molecular dynamics study of the material property changes induced by accumulated point defects in graphite. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2019 , 455, 52-56	1.2	3
66	Release of helium-related clusters through a nickel-graphene interface: An atomistic study. <i>Applied Surface Science</i> , 2019 , 487, 218-227	6.7	3
65	Evaluation of tungsten interatomic potentials for radiation damage simulations. <i>Tungsten</i> , 2020 , 2, 3-14	4.6	3
64	Ab initio-based Er-Fe interatomic potential in hcp Er. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2014 , 22, 065009	2	3
63	Theory of suppressing avalanche process of carrier in short pulse laser irradiated dielectrics. <i>Journal of Applied Physics</i> , 2014 , 115, 203112	2.5	3
62	Cu Segregation at Σ Symmetrical Grain Boundary in δ -Fe: Atomic-Level Simulations. <i>Chinese Physics Letters</i> , 2014 , 31, 096801	1.8	3
61	Radiation response of inorganic scintillators: insights from Monte Carlo simulations 2014 ,		3
60	Ab initio Study of He Stability in hcp α -Ti. <i>Chinese Physics Letters</i> , 2010 , 27, 123102	1.8	3
59	The influence of a surface on defect production by 10 keV displacement cascades in Ni ₃ Al. <i>Radiation Effects and Defects in Solids</i> , 1997 , 141, 395-407	0.9	3
58	Molecular dynamics simulation of low-energy recoil events in titanate pyrochlores. <i>RSC Advances</i> , 2017 , 7, 35403-35410	3.7	3
57	Analytical bond-order potential for silver, palladium, ruthenium and iodine bulk diffusion in silicon carbide. <i>Journal of Physics Condensed Matter</i> , 2020 , 32, 085702	1.8	3
56	Study on the mechanism of helium platelets formation at low temperatures in SiC from the perspective of atomic diffusion. <i>Journal of Nuclear Materials</i> , 2020 , 542, 152507	3.3	3
55	Does the Mg ₁₂ Battery Suffer Severe Shuttle Effect?. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 28518-28527	3.5	3
54	Low energy ion-solid interactions and chemistry effects in a series of pyrochlores. <i>Journal of the American Ceramic Society</i> , 2017 , 100, 3132-3144	3.8	2

53	First-Principles Assessment of the Structure and Stability of 15 Intrinsic Point Defects in Zinc-Blende Indium Arsenide. <i>Crystals</i> , 2019 , 9, 48	2:3	2
52	High Performance SiGe Body-On-Insulator (BOI) FinFET Fabricated on Bulk Si Substrate Using Ge Condensation Technique. <i>IEEE Electron Device Letters</i> , 2020 , 41, 1280-1283	4:4	2
51	Anisotropic Migration of Defects under Strain Effect in BCC Iron. <i>Chinese Physics Letters</i> , 2017 , 34, 0761028		2
50	Many-Body Theory of Proton-Generated Point Defects for Losses of Electron Energy and Photons in Quantum Wells. <i>Physical Review Applied</i> , 2018 , 9,	4:3	2
49	Wetting characteristics of lithium droplet on iron surfaces in atomic scale: A molecular dynamics simulation. <i>Computational Materials Science</i> , 2018 , 149, 435-441	3:2	2
48	Effect of neon on the hydrogen behaviors in tungsten: A first-principles study. <i>Journal of Nuclear Materials</i> , 2018 , 510, 492-498	3:3	2
47	Modified analytic embedded atom method potential for chromium. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2018 , 26, 065001	2	2
46	Migration of defect clusters and xenon-vacancy clusters in uranium dioxide. <i>International Journal of Modern Physics B</i> , 2014 , 28, 1450120	1:1	2
45	Ab initio calculations of mechanical properties in ErM_2Hex (M = Er, Sc). <i>European Physical Journal B</i> , 2014 , 87, 1	1:2	2
44	Defects and Doping in One-Dimensional SiC Nanostructures. <i>Journal of Computational and Theoretical Nanoscience</i> , 2012 , 9, 1967-1974	0:3	2
43	Vacancies in fully hydrogenated boron nitride layer: implications for functional nanodevices. <i>Physica Status Solidi - Rapid Research Letters</i> , 2012 , 6, 105-107	2:5	2
42	Tungsten cluster migration on nanoparticles: minimum energy pathway and migration mechanism. <i>European Physical Journal B</i> , 2011 , 80, 31-40	1:2	2
41	Dual-donor codoping approach to realize low-resistance n-type ZnS semiconductor. <i>Applied Physics Letters</i> , 2011 , 99, 052109	3:4	2
40	Stability of S and Se induced reconstructions on GaP(001)(2 \times 1) surface. <i>Physica B: Condensed Matter</i> , 2010 , 405, 4262-4266	2:8	2
39	Thermodynamic Assessment of Phase Equilibria in the Sn-Ag-Ni System with Key Experimental Verification. <i>Journal of Electronic Materials</i> , 2008 , 37, 279-287	1:9	2
38	Low-energy sputtering events at free surfaces near anti-phase and grain boundaries in Ni ₃ Al. <i>Philosophical Magazine</i> , 2006 , 86, 4243-4258	1:6	2
37	MD Investigation of Thermal Spike Effects on Defect Production and Disorder by Displacement Cascades in Ni ₃ Al. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 540, 661		2
36	Computer Simulation of Displacement Cascades in Zr . <i>Materials Research Society Symposia Proceedings</i> , 1996 , 439, 395		2

35	Molecular dynamics simulation of the interactions between screw dislocation and stacking fault tetrahedron in Fe ₁₀ Ni ₂₀ Cr and Ni. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2020 , 28, 075002	2	2
34	Effect of H on the formation of vacancy dislocation loops in Fe. <i>Journal of Nuclear Materials</i> , 2020 , 542, 152500	3.3	2
33	Atomistic simulation of displacement damage and effective nonionizing energy loss in InAs. <i>Physical Review Materials</i> , 2021 , 5,	3.2	2
32	Analytical interatomic potential for a molybdenum-beryllium system. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2016 , 24, 045018	2	2
31	Non-thermal melting of tungsten under intense electronic excitations. <i>Acta Materialia</i> , 2021 , 216, 117158.4	5.4	2
30	Machine learning to predict aluminum segregation to magnesium grain boundaries. <i>Scripta Materialia</i> , 2021 , 204, 114150	5.6	2
29	Stability and physical properties tuning via interstitials chemical engineering of Zr ₅ Sn ₃ : a first-principles study. <i>Journal of Materials Science</i> , 2019 , 54, 10284-10296	4.3	1
28	A first-principles study of the avalanche pressure of alpha zirconium. <i>RSC Advances</i> , 2016 , 6, 72551-72558.7	5.7	1
27	Measuring the complex admittance and tunneling rate of a germanium hut wire hole quantum dot. <i>Journal of Applied Physics</i> , 2018 , 123, 174305	2.5	1
26	Helium nano-bubble bursting near the nickel surface. <i>Chinese Physics B</i> , 2017 , 26, 113401	1.2	1
25	Multi-Timescale Microscopic Theory for Radiation Degradation of Electronic and Optoelectronic Devices. <i>Space Science International</i> , 2015 , 3, 3-27		1
24	Integrated Material System Modeling of Fusion Blanket. <i>Materials Transactions</i> , 2013 , 54, 477-483	1.3	1
23	First principles study of p-type doping in SiC nanowires: role of quantum effect. <i>Journal of Nanoparticle Research</i> , 2011 , 13, 2887-2892	2.3	1
22	Molecular dynamic simulations of displacement cascades in tungsten and tungsten-beryllium alloys: Effects of grain boundary and/or phase. <i>Journal of Nuclear Materials</i> , 2022 , 561, 153543	3.3	1
21	Temperature effects on defect production and disordering by displacement cascades in Ni ₃ Al		1
20	Clustering and dislocation loop punching induced by different noble gas bubbles in tungsten: a molecular dynamics study. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019 , 27, 084002	2.2	0
19	Reduction of defect generation and development of sinks at nanocluster boundary in oxide dispersion-strengthened steel. <i>Journal of Applied Physics</i> , 2019 , 126, 084302	2.5	0
18	Monte Carlo simulation of the passage of rays and particles in CsI. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2021 , 490, 25-33	1.2	0

17	Dynamics of defect-loaded grain boundary under shear deformation in alpha iron. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2018 , 26, 025006	2	o
16	Strong interfacial coupling in vertical WSe ₂ /WS ₂ heterostructure for high performance photodetection. <i>Applied Physics Letters</i> , 2022 , 120, 181108	3.4	o
15	Orientation dependence of shock-induced change of habit plane for the 1/2<111> dislocation loop and plasticity in tungsten. <i>International Journal of Plasticity</i> , 2022 , 155, 103329	7.6	o
14	Nanowires: Site-Controlled Uniform Ge/Si Heterostructures with Electrically Tunable Spin-Orbit Coupling (Adv. Mater. 16/2020). <i>Advanced Materials</i> , 2020 , 32, 2070122	24	
13	An Isotropic Empirical Intermolecular Potential for Solid H ₂ and D ₂ : A Classical Molecular Calculation. <i>Chinese Physics Letters</i> , 2017 , 34, 123401	1.8	
12	Effect of vacancies on the nucleation of Cr precipitates at grain boundary in Fe. <i>Canadian Journal of Physics</i> , 2019 , 97, 842-846	1.1	
11	Molecular Dynamics Simulation of Thermodynamic Properties in Uranium Dioxide. <i>Nuclear Science and Engineering</i> , 2014 , 176, 360-369	1.2	
10	Precipitates of Cr at B {112} GB in Fe. <i>Materials Research Society Symposia Proceedings</i> , 2014 , 1645, 1		
9	Surface Structure and Electronic Property of Sulfur Passivation of InAs(001) Surface: A First-Principles Study. <i>Materials Science Forum</i> , 2011 , 689, 220-225	0.4	
8	In-Situ TEM Study of Phase Transformation and Structural Evolution of Si-C Nanocomposite Anode for Lithium Ion Battery. <i>Microscopy and Microanalysis</i> , 2012 , 18, 1320-1321	0.5	
7	Computer Simulation of Defect Production and Behaviour in Displacement Cascades in Metals. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 538, 127		
6	Ab initio investigation of properties and mobility of helium defects in La ₂ Sn ₂ O ₇ pyrochlore. <i>Nuclear Materials and Energy</i> , 2022 , 30, 101135	2.1	
5	Abnormal radiation resistance via direct-amorphization-induced defect recovery in HgTe. <i>Applied Physics Letters</i> , 2022 , 120, 012101	3.4	
4	Energetics and Length Scales of Point Defect and Element Segregation to Grain Boundaries in Fe ₇₂ Cr ₂₈		
3	Atomistic study on helium-to-vacancy ratio of neutron irradiation induced helium bubbles during nucleation and growth in Fe. <i>Nuclear Materials and Energy</i> , 2021 , 26, 100940	2.1	
2	Assessing Atomic-Phase Transitions and Ion Transport in Layered Na _x NiO ₂ (x = 0.67) Cathode Materials. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 4930-4937	3.8	
1	Manipulating Picosecond Photoresponse in van der Waals Heterostructure Photodetectors. <i>Advanced Functional Materials</i> , 2020 , 30, 200973	15.6	