

Christophe Domain

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175
papers

8,362
citations

49
h-index

87
g-index

181
ext. papers

9,048
ext. citations

3.3
avg, IF

6.17
L-index

#	Paper	IF	Citations
175	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. <i>Journal of Nuclear Materials</i> , 2013 , 432, 482-500	3.3	494
174	Ab initio calculations of defects in Fe and dilute Fe-Cu alloys. <i>Physical Review B</i> , 2001 , 65,	3.3	346
173	Ab initio study of foreign interstitial atom (C, N) interactions with intrinsic point defects in α -Fe. <i>Physical Review B</i> , 2004 , 69,	3.3	312
172	Density functional theory analysis of the structural and electronic properties of TiO ₂ rutile and anatase polytypes: performances of different exchange-correlation functionals. <i>Journal of Chemical Physics</i> , 2007 , 126, 154703	3.9	276
171	Simulation of radiation damage in Fe alloys: an object kinetic Monte Carlo approach. <i>Journal of Nuclear Materials</i> , 2004 , 335, 121-145	3.3	243
170	Migration energy of He in W revisited by ab initio calculations. <i>Physical Review Letters</i> , 2006 , 97, 196402	7.4	241
169	Ab initio study of Cr interactions with point defects in bcc Fe. <i>Physical Review B</i> , 2007 , 75,	3.3	239
168	Simulation of screw dislocation motion in iron by molecular dynamics simulations. <i>Physical Review Letters</i> , 2005 , 95, 215506	7.4	183
167	Comparison of empirical interatomic potentials for iron applied to radiation damage studies. <i>Journal of Nuclear Materials</i> , 2010 , 406, 19-38	3.3	179
166	Optimisation of accurate rutile TiO ₂ (110), (100), (101) and (001) surface models from periodic DFT calculations. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 565-574	1.9	179
165	Ab initio calculations about intrinsic point defects and He in W. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 255, 23-26	1.2	178
164	Two-band modeling of δ prime phase formation in Fe-Cr. <i>Physical Review B</i> , 2005 , 72,	3.3	175
163	Ab initio study of solute transition-metal interactions with point defects in bcc Fe. <i>Physical Review B</i> , 2010 , 81,	3.3	173
162	Atomistic modeling of an Fe system with a small concentration of C. <i>Computational Materials Science</i> , 2007 , 40, 119-129	3.2	148
161	An object Kinetic Monte Carlo Simulation of the dynamics of helium and point defects in tungsten. <i>Journal of Nuclear Materials</i> , 2009 , 385, 223-227	3.3	147
160	Microstructural evolution of irradiated tungsten: Ab initio parameterisation of an OKMC model. <i>Journal of Nuclear Materials</i> , 2010 , 403, 75-88	3.3	146
159	Review on the EFDA programme on tungsten materials technology and science. <i>Journal of Nuclear Materials</i> , 2011 , 417, 463-467	3.3	139

158	Combined investigation of water sorption on TiO ₂ rutile (1 1 0) single crystal face: XPS vs. periodic DFT. <i>Surface Science</i> , 2007 , 601, 518-527	1.8	137
157	Atomic-scale Ab-initio study of the Zr-H system: I. Bulk properties. <i>Acta Materialia</i> , 2002 , 50, 3513-3526	8.4	133
156	Exact ab initio transport coefficients in bcc Fe \bar{X} (X=Cr, Cu, Mn, Ni, P, Si) dilute alloys. <i>Physical Review B</i> , 2014 , 90,	3.3	122
155	A density functional theory assessment of the clustering behaviour of He and H in tungsten. <i>Journal of Nuclear Materials</i> , 2009 , 386-388, 109-111	3.3	117
154	Influence of the interatomic potentials on molecular dynamics simulations of displacement cascades. <i>Journal of Nuclear Materials</i> , 2000 , 280, 73-85	3.3	114
153	Mean field rate theory and object kinetic Monte Carlo: A comparison of kinetic models. <i>Journal of Nuclear Materials</i> , 2008 , 382, 77-90	3.3	112
152	Ab initio modelling of defect properties with substitutional and interstitials elements in steels and Zr alloys. <i>Journal of Nuclear Materials</i> , 2006 , 351, 1-19	3.3	86
151	Recent advances in modeling and simulation of the exposure and response of tungsten to fusion energy conditions. <i>Nuclear Fusion</i> , 2017 , 57, 092008	3.3	85
150	Self-trapped interstitial-type defects in iron. <i>Physical Review Letters</i> , 2008 , 100, 145503	7.4	84
149	Solute interaction with point defects in β Fe during thermal ageing: A combined ab initio and atomic kinetic Monte Carlo approach. <i>Journal of Nuclear Materials</i> , 2006 , 351, 88-99	3.3	84
148	Precipitation of the FeCu system: A critical review of atomic kinetic Monte Carlo simulations. <i>Journal of Nuclear Materials</i> , 2008 , 373, 387-401	3.3	80
147	Solute-point defect interactions in bcc systems: Focus on first principles modelling in W and RPV steels. <i>Current Opinion in Solid State and Materials Science</i> , 2012 , 16, 115-125	12	75
146	Ab initio investigation of potential indium and gallium free chalcopyrite compounds for photovoltaic application. <i>Journal of Physics and Chemistry of Solids</i> , 2005 , 66, 2019-2023	3.9	75
145	Diffusion of phosphorus in β Fe: An ab initio study. <i>Physical Review B</i> , 2005 , 71,	3.3	74
144	Atomic-scale ab initio study of the Zr-H system: II. Interaction of H with plane defects and mechanical properties. <i>Acta Materialia</i> , 2004 , 52, 1495-1502	8.4	74
143	Ab initio atomic-scale determination of point-defect structure in hcp zirconium. <i>Philosophical Magazine</i> , 2005 , 85, 569-575	1.6	68
142	Ab initio calculations and interatomic potentials for iron and iron alloys: Achievements within the Perfect Project. <i>Journal of Nuclear Materials</i> , 2010 , 406, 7-18	3.3	67
141	Structural investigation and electronic properties of the nickel ferrite NiFe ₂ O ₄ : a periodic density functional theory approach. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 346219	1.8	67

140	Formation and evolution of MnNi clusters in neutron irradiated dilute Fe alloys modelled by a first principle-based AKMC method. <i>Journal of Nuclear Materials</i> , 2012 , 426, 198-207	3-3	66
139	Kinetics of G-phase precipitation and spinodal decomposition in very long aged ferrite of a Mo-free duplex stainless steel. <i>Journal of Nuclear Materials</i> , 2015 , 465, 383-389	3-3	64
138	A brief summary of the progress on the EFDA tungsten materials program. <i>Journal of Nuclear Materials</i> , 2013 , 442, S173-S180	3-3	63
137	Object kinetic Monte Carlo study of sink strengths. <i>Journal of Nuclear Materials</i> , 2007 , 360, 159-169	3-3	62
136	Ab initio contribution to the study of complexes formed during dilute FeCu alloys radiation. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2003 , 202, 44-50	1.2	62
135	Modeling the long-term evolution of the primary damage in ferritic alloys using coarse-grained methods. <i>Journal of Nuclear Materials</i> , 2010 , 406, 39-54	3-3	61
134	Ab initio calculations of self-interstitial interaction and migration with solute atoms in bcc Fe. <i>Journal of Nuclear Materials</i> , 2006 , 359, 227-237	3-3	61
133	Ab initio calculations of vacancy interactions with solute atoms in bcc Fe. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2005 , 228, 137-141	1.2	60
132	Helium self-interstitial atom interaction in Iron. <i>Journal of Nuclear Materials</i> , 2006 , 351, 119-132	3-3	59
131	Atomistic Kinetic Monte Carlo studies of microchemical evolutions driven by diffusion processes under irradiation. <i>Journal of Nuclear Materials</i> , 2010 , 406, 55-67	3-3	57
130	Kinetic study of phase transformation in a highly concentrated FeCr alloy: Monte Carlo simulation versus experiments. <i>Acta Materialia</i> , 2011 , 59, 2404-2411	8.4	56
129	Ab initio threshold displacement energies in iron. <i>Materials Research Letters</i> , 2016 , 4, 219-225	7.4	53
128	Microstructural evolution under high flux irradiation of dilute FeCuNiMnSi alloys studied by an atomic kinetic Monte Carlo model accounting for both vacancies and self interstitials. <i>Journal of Nuclear Materials</i> , 2008 , 382, 154-159	3-3	50
127	Modelling self trapping and trap mutation in tungsten using DFT and Molecular Dynamics with an empirical potential based on DFT. <i>Journal of Nuclear Materials</i> , 2014 , 455, 10-15	3-3	49
126	Self-interstitial defects in hexagonal close packed metals revisited: Evidence for low-symmetry configurations in Ti, Zr, and Hf. <i>Physical Review B</i> , 2013 , 87,	3-3	49
125	Modeling Microstructure and Irradiation Effects. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2011 , 42, 852-870	2-3	49
124	Atomic kinetic Monte Carlo model based on ab initio data: Simulation of microstructural evolution under irradiation of dilute FeCuNiMnSi alloys. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 255, 78-84	1.2	47
123	Non-equilibrium properties of interatomic potentials in cascade simulations in tungsten. <i>Journal of Nuclear Materials</i> , 2016 , 470, 119-127	3-3	46

122	Ab initio calculation of intrinsic point defects in CuInSe ₂ . <i>Journal of Physics and Chemistry of Solids</i> , 2003 , 64, 1657-1663	3.9	46
121	The role of Cu in displacement cascades examined by molecular dynamics. <i>Journal of Nuclear Materials</i> , 2001 , 294, 274-287	3.3	46
120	First-principles study of point defects in an fcc Fe-10Ni-20Cr model alloy. <i>Physical Review B</i> , 2014 , 89,	3.3	44
119	Ferromagnetic compounds for high efficiency photovoltaic conversion: the case of AlP:Cr. <i>Physical Review Letters</i> , 2009 , 102, 227204	7.4	43
118	Dependence of radiation damage accumulation in iron on underlying models of displacement cascades and subsequent defect migration. <i>Journal of Nuclear Materials</i> , 2006 , 355, 89-103	3.3	43
117	Atomic displacement cascade distributions in iron. <i>Journal of Nuclear Materials</i> , 2001 , 295, 179-188	3.3	42
116	Comparison of atomistic and elasticity approaches for carbon diffusion near line defects in Iron. <i>Acta Materialia</i> , 2011 , 59, 6963-6974	8.4	41
115	Interaction of a 1/2<111> screw dislocation with Cr precipitates in bcc Fe studied by molecular dynamics. <i>Physical Review B</i> , 2010 , 81,	3.3	41
114	Introducing chemistry in atomistic kinetic Monte Carlo simulations of Fe alloys under irradiation. <i>Physica Status Solidi (B): Basic Research</i> , 2010 , 247, 9-22	1.3	40
113	Organic thermoelectric devices based on a stable n-type nanocomposite printed on paper. <i>Sustainable Energy and Fuels</i> , 2018 , 2, 199-208	5.8	38
112	Massively parallel molecular dynamics simulations with EAM potentials. <i>Radiation Effects and Defects in Solids</i> , 1997 , 142, 9-21	0.9	38
111	TEM investigations of the oxide layers formed on a 316L alloy in simulated PWR environment. <i>Journal of Materials Science</i> , 2013 , 48, 2861-2871	4.3	37
110	Effect of the stress field of an edge dislocation on carbon diffusion in Iron: Coupling molecular statics and atomistic kinetic Monte Carlo. <i>Physical Review B</i> , 2010 , 82,	3.3	37
109	Microstructure evolution of irradiated tungsten: Crystal effects in He and H implantation as modelled in the Binary Collision Approximation. <i>Journal of Nuclear Materials</i> , 2010 , 403, 89-100	3.3	34
108	Stability and mobility of small vacancy and copper-vacancy clusters in bcc-Fe: An atomistic kinetic Monte Carlo study. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 255, 47-51	1.2	31
107	Effect of displacement cascade structure and defect mobility on the growth of point defect clusters under irradiation. <i>Journal of Nuclear Materials</i> , 2006 , 351, 39-46	3.3	31
106	Mechanisms of radiation strengthening in Fe-Cr alloys as revealed by atomistic studies. <i>Journal of Nuclear Materials</i> , 2013 , 442, 470-485	3.3	30
105	First principle-based AKMC modelling of the formation and medium-term evolution of point defect and solute-rich clusters in a neutron irradiated complex Fe-Cu-Mn-Ni-Si-P alloy representative of reactor pressure vessel steels. <i>Journal of Nuclear Materials</i> , 2013 , 440, 143-152	3.3	30

104	Theoretical investigation of the uranyl ion sorption on the rutile TiO ₂ (110) face. <i>Inorganic Chemistry</i> , 2008 , 47, 10991-7	5.1	30
103	Multiscale modelling of the interaction of hydrogen with interstitial defects and dislocations in BCC tungsten. <i>Nuclear Fusion</i> , 2018 , 58, 016006	3.3	29
102	Solute $\langle 111 \rangle$ interstitial loop interaction in α -Fe: A DFT study. <i>Journal of Nuclear Materials</i> , 2018 , 499, 582-594	3.3	29
101	Modeling of the self trapping of helium and the trap mutation in tungsten using DFT and empirical potentials based on DFT. <i>Journal of Materials Research</i> , 2014 , 29, 2374-2386	2.5	28
100	Periodic density functional theory investigation of the uranyl ion sorption on the TiO ₂ rutile (110) face. <i>Inorganic Chemistry</i> , 2006 , 45, 6568-70	5.1	28
99	Vacancy-solute complexes and their clusters in iron. <i>Applied Surface Science</i> , 2006 , 252, 3303-3308	6.7	28
98	Interactions between dislocations and irradiation-induced defects in light water reactor pressure vessel steels. <i>Journal of Nuclear Materials</i> , 2005 , 346, 79-97	3.3	28
97	Quantitative phase field model for dislocation sink strength calculations. <i>Computational Materials Science</i> , 2014 , 88, 50-60	3.2	27
96	On the correlation between primary damage and long-term nanostructural evolution in iron under irradiation. <i>Journal of Nuclear Materials</i> , 2011 , 419, 122-133	3.3	27
95	Short- and long-range orders in FeCr: A Monte Carlo study. <i>Journal of Applied Physics</i> , 2009 , 106, 104906	2.5	27
94	Comparison between three complementary approaches to simulate large fluence irradiation: application to electron irradiation of thin foils. <i>Philosophical Magazine</i> , 2005 , 85, 541-547	1.6	27
93	Quantification of hardening contribution of G-Phase precipitation and spinodal decomposition in aged duplex stainless steel: APT analysis and micro-hardness measurements. <i>Journal of Nuclear Materials</i> , 2019 , 514, 266-275	3.3	27
92	Simulation of Irradiation Effects in Reactor Pressure Vessel Steels: the Reactor for Virtual Experiments (REVE) Project. <i>Journal of Testing and Evaluation</i> , 2002 , 30, 37	1	26
91	Fe-doped CuInSe ₂ : An ab initio study of magnetic defects in a photovoltaic material. <i>Physical Review B</i> , 2005 , 71,	3.3	25
90	Atomistic modeling of carbon Cottrell atmospheres in bcc iron. <i>Journal of Physics Condensed Matter</i> , 2013 , 25, 025401	1.8	23
89	Sink strength calculations of dislocations and loops using OKMC. <i>Journal of Nuclear Materials</i> , 2013 , 442, 218-226	3.3	23
88	Investigation of hydrogen bonds and temperature effects on the water monolayer adsorption on rutile TiO ₂ (110) by first-principles molecular dynamics simulations. <i>Surface Science</i> , 2011 , 605, 1275-1280	1.8	23
87	Kinetic Monte Carlo Simulations of FeCu Alloys. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 540, 643		23

86	Isochronal annealing of electron-irradiated dilute Fe alloys modelled by an ab initio based AKMC method: Influence of soluteInterstitial cluster properties. <i>Journal of Nuclear Materials</i> , 2010 , 407, 16-28	3.3	22
85	Kinetics of secondary phase precipitation during spinodal decomposition in duplex stainless steels: A kinetic Monte Carlo model Comparison with atom probe tomography experiments. <i>Journal of Nuclear Materials</i> , 2014 , 451, 361-365	3.3	21
84	Improved atomistic Monte Carlo models based on ab-initio-trained neural networks: Application to FeCu and FeCr alloys. <i>Physical Review B</i> , 2017 , 95,	3.3	20
83	Overview of the RPV-2 and INTERN-1 packages: From primary damage to microplasticity. <i>Journal of Nuclear Materials</i> , 2010 , 406, 175-186	3.3	20
82	Modelling of Radiation Damage in Fe-Cr Alloys. <i>Journal of ASTM International</i> , 2007 , 4, 100692		20
81	The impact of alloying elements on the precipitation stability and kinetics in iron based alloys: An atomistic study. <i>Computational Materials Science</i> , 2019 , 161, 309-320	3.2	19
80	Theoretical first step towards an understanding of the uranyl ion sorption on the rutile TiO ₂ (110) face: A DFT periodic and cluster study. <i>Radiochimica Acta</i> , 2006 , 94, 601-607	1.9	18
79	Ab initio calculations of some atomic and point defect interactions involving C and N in Fe. <i>Philosophical Magazine</i> , 2005 , 85, 533-540	1.6	18
78	Modeling of helium bubble nucleation and growth in austenitic stainless steels using an Object Kinetic Monte Carlo method. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2015 , 352, 107-114	1.2	17
77	Advanced atomistic models for radiation damage in Fe-based alloys: Contributions and future perspectives from artificial neural networks. <i>Computational Materials Science</i> , 2018 , 148, 116-130	3.2	17
76	Effect of the applied stress and the friction stress on the dislocation dissociation in face centered cubic metals. <i>Materials Letters</i> , 2013 , 97, 93-96	3.3	17
75	A DFT study of the stability of SIAs and small SIA clusters in the vicinity of solute atoms in Fe. <i>Journal of Nuclear Materials</i> , 2018 , 500, 92-109	3.3	17
74	Introducing ab initio based neural networks for transition-rate prediction in kinetic Monte Carlo simulations. <i>Physical Review B</i> , 2017 , 95,	3.3	16
73	Structure of nanoscale copper precipitates in neutron-irradiated Fe-Cu-C alloys. <i>Physical Review B</i> , 2012 , 85,	3.3	16
72	Relevancy of displacement cascades features to the long term point defect cluster growth. <i>Journal of Nuclear Materials</i> , 2008 , 382, 103-111	3.3	16
71	Atomic structure of grain boundaries in iron modeled using the atomic density function. <i>Physical Review B</i> , 2014 , 89,	3.3	15
70	Vacancy migration energy dependence on local chemical environment in FeCr alloys: A Density Functional Theory study. <i>Journal of Nuclear Materials</i> , 2014 , 452, 425-433	3.3	15
69	Interatomic potential to study the formation of NiCr clusters in high Cr ferritic steels. <i>Journal of Nuclear Materials</i> , 2017 , 484, 42-50	3.3	15

68	Influence of shape anisotropy of self-interstitials on dislocation sink efficiencies in Zr: Multiscale modeling. <i>Physical Review B</i> , 2014 , 90,	3.3	15
67	Further development of large-scale atomistic modelling techniques for Fe/Cr alloys. <i>Journal of Nuclear Materials</i> , 2011 , 409, 167-175	3.3	15
66	Nanostructure evolution under irradiation of Fe(C)MnNi model alloys for reactor pressure vessel steels. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2015 , 352, 56-60	1.2	14
65	A new scenario for γ -vacancy loop formation in zirconium based on atomic-scale modeling. <i>Acta Materialia</i> , 2019 , 179, 93-106	8.4	13
64	Recent radiation damage studies and developments of the Marlowe code. <i>Radiation Effects and Defects in Solids</i> , 2014 , 169, 592-602	0.9	13
63	First-principles molecular dynamics simulations of uranyl ion interaction at the water/rutile TiO ₂ (110) interface. <i>Surface Science</i> , 2012 , 606, 1135-1141	1.8	13
62	Copper precipitation in iron: a comparison between metropolis Monte Carlo and lattice kinetic Monte Carlo methods. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2003 , 202, 68-75	1.2	13
61	Primary damage in tungsten using the binary collision approximation, molecular dynamic simulations and the density functional theory. <i>Physica Scripta</i> , 2016 , T167, 014018	2.6	12
60	Ab initio atomic-scale modelling of iodine effects on hcp zirconium. <i>Philosophical Magazine</i> , 2005 , 85, 589-595	1.6	12
59	The influence of the internal displacement cascades structure on the growth of point defect clusters in radiation environment. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2005 , 228, 181-186	1.2	12
58	Flexible thermoelectric device based on TiS ₂ (HA) _x n-type nanocomposite printed on paper. <i>Organic Electronics</i> , 2019 , 68, 256-263	3.5	12
57	The dominant mechanisms for the formation of solute-rich clusters in low-Cu steels under irradiation. <i>Materials Today Energy</i> , 2020 , 17, 100472	7	11
56	Anti-aging treatment of nuclear power plant steel. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2018 , 735, 73-80	5.3	11
55	Atomic and dislocation dynamics simulations of plastic deformation in reactor pressure vessel steel. <i>Journal of Nuclear Materials</i> , 2009 , 394, 174-181	3.3	11
54	Investigation of solute segregation behavior using a correlative EBSD/TKD/APT methodology in a 16MND5 weld. <i>Journal of Nuclear Materials</i> , 2019 , 523, 434-443	3.3	10
53	Molecular dynamics investigation of the interaction of an edge dislocation with Frank loops in Fe ₈₀ Ni ₁₀ Cr ₂₀ alloy. <i>Journal of Nuclear Materials</i> , 2015 , 465, 301-310	3.3	10
52	The topological skeleton of cellular automaton dynamics. <i>Physica D: Nonlinear Phenomena</i> , 1997 , 103, 155-168	3.3	10
51	Elastic dipole tensors and relaxation volumes of point defects in concentrated random magnetic Fe-Cr alloys. <i>Computational Materials Science</i> , 2021 , 194, 110435	3.2	10

50	Influence of vacancy diffusional anisotropy: Understanding the growth of zirconium alloys under irradiation and their microstructure evolution. <i>Acta Materialia</i> , 2020 , 195, 631-644	8.4	9
49	A model of defect cluster creation in fragmented cascades in metals based on morphological analysis. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 405701	1.8	9
48	Hydrogen accumulation around dislocation loops and edge dislocations: from atomistic to mesoscopic scales in BCC tungsten. <i>Physica Scripta</i> , 2017 , T170, 014073	2.6	9
47	Density functional theory-based cluster expansion to simulate thermal annealing in FeCrW alloys. <i>Philosophical Magazine</i> , 2017 , 97, 299-317	1.6	9
46	Comparison of algorithms for multiscale modelling of radiation damage in FeCu alloys. <i>Philosophical Magazine</i> , 2005 , 85, 417-428	1.6	9
45	Uranyl interaction with the hydrated (1 1 1) nickel face: A periodic density functional theory investigation. <i>Surface Science</i> , 2008 , 602, 3331-3337	1.8	8
44	State of Advancement of the International REVE Project: Computational Modelling of Irradiation-Induced Hardening in Reactor Pressure Vessel Steels and Relevant Experimental Validation Programme 2002 , 267		7
43	Kinetic Monte Carlo simulations of cascades in Fe alloys. <i>Materials Research Society Symposia Proceedings</i> , 2000 , 650, 3251		7
42	Numerical evaluation of dislocation loop sink strengths: A phase-field approach. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2015 , 352, 31-35	1.2	6
41	Carbon diffusion in bulk hcp zirconium: A multi-scale approach. <i>Journal of Nuclear Materials</i> , 2016 , 473, 61-67	3.3	6
40	Kinetic Monte Carlo Simulations of FeCu Alloys. <i>Materials Research Society Symposia Proceedings</i> , 1998 , 538, 217		6
39	Thermodynamic modeling of G-phase and assessment of phase stabilities in reactor pressure vessel steels and cast duplex stainless steels. <i>Journal of Nuclear Materials</i> , 2020 , 533, 152091	3.3	5
38	Kinetic Monte Carlo simulation of nanostructural evolution under post-irradiation annealing in dilute FeMnNi. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2015 , 12, 20-24		5
37	Computer simulations study of iron-copper alloy. <i>Radiation Effects and Defects in Solids</i> , 1997 , 141, 325-336		5
36	Solute-point defect interactions, coupled diffusion, and radiation-induced segregation in fcc nickel. <i>Physical Review Materials</i> , 2021 , 5,	3.2	5
35	Investigation of Glide Properties in Hexagonal Titanium and Zirconium: An Ab Initio Atomic Scale Study. <i>Solid Mechanics and Its Applications</i> , 2004 , 411-420	0.4	5
34	Spatial effects in the 800keV 3He implantation in W followed by isochronal annealing at 900K. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2013 , 303, 87-90	1.2	4
33	Uranyl ion interaction at the water/NiO(100) interface: a predictive investigation by first-principles molecular dynamic simulations. <i>Journal of Chemical Physics</i> , 2012 , 137, 164701	3.9	4

32	Molecular dynamics simulations of damage and plasticity: The role of ab initio calculations in the development of interatomic potentials. <i>Philosophical Magazine</i> , 2009 , 89, 3215-3234	1.6	4
31	Towards improved photovoltaic conversion using dilute magnetic semiconductors (abstract only). <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 064226	1.8	4
30	Kinetic Monte Carlo Simulations of Irradiation Effects 2020 , 754-778		4
29	Effect of annealing treatment at 550 °C on ferrite of thermally aged cast austenitic stainless steels and ageing kinetics of reverted cast austenitic stainless steels. <i>Journal of Nuclear Materials</i> , 2020 , 542, 152530	3.3	4
28	Influence of Ni, Mo and Mn Content on the G-Phase Precipitation and Spinodal Decomposition of Aged Duplex Stainless Steels.. <i>Microscopy and Microanalysis</i> , 2017 , 23, 728-729	0.5	3
27	Phase-field calculations of sink strength in Al, Ni, and Fe: A detailed study of elastic effects. <i>Computational Materials Science</i> , 2020 , 183, 109905	3.2	3
26	Physical mechanisms and parameters for models of microstructure evolution under irradiation in Fe alloys [Part I: Pure Fe. <i>Nuclear Materials and Energy</i> , 2021 , 29, 101069	2.1	3
25	Sintering of ferritic and austenitic nanopowders using Spark Plasma Sintering. <i>Metallurgical Research and Technology</i> , 2014 , 111, 305-310	0.9	2
24	Simulation of the irradiation effects in reactor materials : The REVE project. <i>European Physical Journal Special Topics</i> , 2000 , 10, Pr6-191-Pr6-196		2
23	Effect of Ni, Mo and Mn content on spinodal decomposition kinetics and G-phase precipitation of aged model cast austenitic stainless steels. <i>Journal of Nuclear Materials</i> , 2021 , 555, 153123	3.3	2
22	Long term simulation of point defect cluster size distributions from atomic displacement cascades in Fe 70 Cr 20 Ni 10. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2015 , 352, 51-55	1.2	1
21	Interaction between interstitial carbon atoms and a $\langle 111 \rangle$ self-interstitial atoms loop in an iron matrix: a combined DFT, off lattice KMC and MD study. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 335901	1.8	1
20	Formation Energies of Point Defects in Copper Indium Diselenide Using ab initio Methods. <i>Materials Research Society Symposia Proceedings</i> , 2003 , 763, 8101		1
19	Molecular Dynamics simulations of displacement cascades: role of the interatomic potentials and of the potential hardening. <i>Materials Research Society Symposia Proceedings</i> , 2000 , 650, 3241		1
18	Impact of the local microstructure fluctuations on radiation-induced segregation in dilute Fe-Ni and Ni-Ti model alloys: A combined modeling and experimental analysis. <i>Acta Materialia</i> , 2021 , 225, 117531	8.4	1
17	Development of a plasticity-oriented interatomic potential for CrFeMnNi high entropy alloys. <i>Computational Materials Science</i> , 2022 , 203, 111165	3.2	1
16	A DFT-driven multifidelity framework for constructing efficient energy models for atomic-scale simulations. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2020 , 483, 15-21	1.2	1
15	Study of solute segregation behavior at carbide/ferrite interfaces in 16MND5 welds. <i>Journal of Nuclear Materials</i> , 2020 , 542, 152531	3.3	1

14	Modelling the primary damage in Fe and W: influence of the short-range interactions on the cascade properties: Part 2 [Multivariate multiple linear regression analysis of displacement cascades. <i>Journal of Nuclear Materials</i> , 2021 , 549, 152887	3.3	1
13	Atomistic Kinetic Monte Carlo and Solute Effects 2018 , 1-20		1
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8	Investigating the kinetics of the formation of a C Cottrell atmosphere around a screw dislocation in bcc iron: a mixed-lattice atomistic kinetic Monte-Carlo analysis. <i>Journal of Physics Condensed Matter</i> , 2021 , 33, 065704	1.8	0
7	Modelling the primary damage in Fe and W: Influence of the short range interactions on the cascade properties: Part 1 [Energy transfer. <i>Journal of Nuclear Materials</i> , 2021 , 547, 152816	3.3	0
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5	Object Kinetic Monte Carlo (OKMC): A Coarse-Grained Approach to Radiation Damage 2020 , 1287-1312		
4	Atomistic Modeling of Radiation Damage in Metallic Alloys 2019 , 673-701		
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1	Atomistic investigation of elementary dislocation properties influencing mechanical behaviour of Cr15Fe46Mn17Ni22 alloy and Cr20Fe70Ni10 alloy. <i>Computational Materials Science</i> , 2022 , 211, 111508	3.2	