Christophe Domain

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Development of a plasticity-oriented interatomic potential for CrFeMnNi high entropy alloys. *Computational Materials Science*, **2022**, 203, 111165	3.2	1
174	Interaction of transmutation products with precipitates, dislocations and grain boundaries in neutron irradiated W. *Materialia*, **2022**, 22, 101370	3.2	1
173	Atomistic investigation of elementary dislocation properties influencing mechanical behaviour of Cr15Fe46Mn17Ni22 alloy and Cr20Fe70Ni10 alloy. *Computational Materials Science*, **2022**, 211, 111508	3.2	
172	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. *Acta Materialia*, **2021**, 225, 117531	8.4	1
171	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. *Journal of Physics Condensed Matter*, **2021**, 33, 065704	1.8	0
170	Modelling the primary damage in Fe and W: Influence of the short range interactions on the cascade properties: Part 1 Energy transfer. *Journal of Nuclear Materials*, **2021**, 547, 152816	3.3	0
169	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. *Journal of Nuclear Materials*, **2021**, 549, 152887	3.3	1
168	Elastic dipole tensors and relaxation volumes of point defects in concentrated random magnetic Fe-Cr alloys. *Computational Materials Science*, **2021**, 194, 110435	3.2	10
167	Solute-point defect interactions, coupled diffusion, and radiation-induced segregation in fcc nickel. *Physical Review Materials*, **2021**, 5,	3.2	5
166	Effect of Ni, Mo and Mn content on spinodal decomposition kinetics and G-phase precipitation of aged model cast austenitic stainless steels. *Journal of Nuclear Materials*, **2021**, 555, 153123	3.3	2
165	Physical mechanisms and parameters for models of microstructure evolution under irradiation in Fe alloys Part I: Pure Fe. *Nuclear Materials and Energy*, **2021**, 29, 101069	2.1	3
164	Influence of vacancy diffusional anisotropy: Understanding the growth of zirconium alloys under irradiation and their microstructure evolution. *Acta Materialia*, **2020**, 195, 631-644	8.4	9
163	Thermodynamic modeling of G-phase and assessment of phase stabilities in reactor pressure vessel steels and cast duplex stainless steels. *Journal of Nuclear Materials*, **2020**, 533, 152091	3.3	5
162	The dominant mechanisms for the formation of solute-rich clusters in low-Cu steels under irradiation. *Materials Today Energy*, **2020**, 17, 100472	7	11
161	Object Kinetic Monte Carlo (OKMC): A Coarse-Grained Approach to Radiation Damage **2020**, 1287-1312		
160	Atomistic Kinetic Monte Carlo and Solute Effects **2020**, 2437-2456		
159	Kinetic Monte Carlo Simulations of Irradiation Effects **2020**, 754-778		4

158	A DFT-driven multifidelity framework for constructing efficient energy models for atomic-scale simulations. *Nuclear Instruments & Methods in Physics Research B*, **2020**, 483, 15-21	1.2	1
157	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. *Journal of Nuclear Materials*, **2020**, 542, 152530	3.3	4
156	Study of solute segregation behavior at carbide–ferrite interfaces in 16MND5 welds. *Journal of Nuclear Materials*, **2020**, 542, 152531	3.3	1
155	Atomic modelling of carbon atom diffusion in monoclinic zirconia volume, subsurface and surface. *Journal of Nuclear Materials*, **2020**, 537, 152193	3.3	
154	Phase-field calculations of sink strength in Al, Ni, and Fe: A detailed study of elastic effects. *Computational Materials Science*, **2020**, 183, 109905	3.2	3
153	Investigation of solute segregation behavior using a correlative EBSD/TKD/APT methodology in a 16MND5 weld. *Journal of Nuclear Materials*, **2019**, 523, 434-443	3.3	10
152	A new scenario for c-vacancy loop formation in zirconium based on atomic-scale modeling. *Acta Materialia*, **2019**, 179, 93-106	8.4	13
151	Atomistic Modeling of Radiation Damage in Metallic Alloys **2019**, 673-701		
150	Flexible thermoelectric device based on TiS2(HA)x n-type nanocomposite printed on paper. *Organic Electronics*, **2019**, 68, 256-263	3.5	12
149	The impact of alloying elements on the precipitation stability and kinetics in iron based alloys: An atomistic study. *Computational Materials Science*, **2019**, 161, 309-320	3.2	19
148	Quantification of hardening contribution of G-Phase precipitation and spinodal decomposition in aged duplex stainless steel: APT analysis and micro-hardness measurements. *Journal of Nuclear Materials*, **2019**, 514, 266-275	3.3	27
147	Advanced atomistic models for radiation damage in Fe-based alloys: Contributions and future perspectives from artificial neural networks. *Computational Materials Science*, **2018**, 148, 116-130	3.2	17
146	Organic thermoelectric devices based on a stable n-type nanocomposite printed on paper. *Sustainable Energy and Fuels*, **2018**, 2, 199-208	5.8	38
145	Multiscale modelling of the interaction of hydrogen with interstitial defects and dislocations in BCC tungsten. *Nuclear Fusion*, **2018**, 58, 016006	3.3	29
144	Interaction between interstitial carbon atoms and a ½ <1 1 1> self-interstitial atoms loop in an iron matrix: a combined DFT, off lattice KMC and MD study. *Journal of Physics Condensed Matter*, **2018**, 30, 335901	1.8	1
143	Anti-aging treatment of nuclear power plant steel. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2018**, 735, 73-80	5.3	11
142	A model of defect cluster creation in fragmented cascades in metals based on morphological analysis. *Journal of Physics Condensed Matter*, **2018**, 30, 405701	1.8	9
141	A DFT study of the stability of SIAs and small SIA clusters in the vicinity of solute atoms in Fe. *Journal of Nuclear Materials*, **2018**, 500, 92-109	3.3	17

140	Solute □<111> interstitial loop interaction in □Fe: A DFT study. *Journal of Nuclear Materials*, **2018**, 499, 582-594	3.3	29
139	Atomistic Kinetic Monte Carlo and Solute Effects **2018**, 1-20		1
138	Object Kinetic Monte Carlo (OKMC): A Coarse-Grained Approach to Radiation Damage **2018**, 1-26		1
137	Atomistic Modeling of Radiation Damage in Metallic Alloys **2018**, 1-30		1
136	Hardening Contribution of G-Phase Nanoparticle Precipitation and Spinodal Decomposition in Aged Duplex Stainless Steel Studied by APT Analysis and Micro-Hardness of Ferrite. *Microscopy and Microanalysis*, **2018**, 24, 2210-2211	0.5	1
135	Introducing ab initio based neural networks for transition-rate prediction in kinetic Monte Carlo simulations. *Physical Review B*, **2017**, 95,	3.3	16
134	Recent advances in modeling and simulation of the exposure and response of tungsten to fusion energy conditions. *Nuclear Fusion*, **2017**, 57, 092008	3.3	85
133	Influence of Ni, Mo and Mn Content on the G-Phase Precipitation and Spinodal Decomposition of Aged Duplex Stainless Steels.. *Microscopy and Microanalysis*, **2017**, 23, 728-729	0.5	3
132	Hydrogen accumulation around dislocation loops and edge dislocations: from atomistic to mesoscopic scales in BCC tungsten. *Physica Scripta*, **2017**, T170, 014073	2.6	9
131	Improved atomistic Monte Carlo models based on ab-initio-trained neural networks: Application to FeCu and FeCr alloys. *Physical Review B*, **2017**, 95,	3.3	20
130	Density functional theory-based cluster expansion to simulate thermal annealing in FeCrW alloys. *Philosophical Magazine*, **2017**, 97, 299-317	1.6	9
129	Interatomic potential to study the formation of NiCr clusters in high Cr ferritic steels. *Journal of Nuclear Materials*, **2017**, 484, 42-50	3.3	15
128	Primary damage in tungsten using the binary collision approximation, molecular dynamic simulations and the density functional theory. *Physica Scripta*, **2016**, T167, 014018	2.6	12
127	Carbon diffusion in bulk hcp zirconium: A multi-scale approach. *Journal of Nuclear Materials*, **2016**, 473, 61-67	3.3	6
126	Non-equilibrium properties of interatomic potentials in cascade simulations in tungsten. *Journal of Nuclear Materials*, **2016**, 470, 119-127	3.3	46
125	Ab initio threshold displacement energies in iron. *Materials Research Letters*, **2016**, 4, 219-225	7.4	53
124	Numerical evaluation of dislocation loop sink strengths: A phase-field approach. *Nuclear Instruments & Methods in Physics Research B*, **2015**, 352, 31-35	1.2	6
123	Kinetics of G-phase precipitation and spinodal decomposition in very long aged ferrite of a Mo-free duplex stainless steel. *Journal of Nuclear Materials*, **2015**, 465, 383-389	3.3	64

122	Long term simulation of point defect cluster size distributions from atomic displacement cascades in Fe 70 Cr 20 Ni 10. *Nuclear Instruments & Methods in Physics Research B*, **2015**, 352, 51-55	1.2	1
121	Nanostructure evolution under irradiation of Fe(C)MnNi model alloys for reactor pressure vessel steels. *Nuclear Instruments & Methods in Physics Research B*, **2015**, 352, 56-60	1.2	14
120	Modeling of helium bubble nucleation and growth in austenitic stainless steels using an Object Kinetic Monte Carlo method. *Nuclear Instruments & Methods in Physics Research B*, **2015**, 352, 107-114	1.2	17
119	Kinetic Monte Carlo simulation of nanostructural evolution under post-irradiation annealing in dilute FeMnNi. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2015**, 12, 20-24		5
118	Molecular dynamics investigation of the interaction of an edge dislocation with Frank loops in FeNi10Cr20 alloy. *Journal of Nuclear Materials*, **2015**, 465, 301-310	3.3	10
117	Modelling self trapping and trap mutation in tungsten using DFT and Molecular Dynamics with an empirical potential based on DFT. *Journal of Nuclear Materials*, **2014**, 455, 10-15	3.3	49
116	Atomic structure of grain boundaries in iron modeled using the atomic density function. *Physical Review B*, **2014**, 89,	3.3	15
115	First-principles study of point defects in an fcc Fe-10Ni-20Cr model alloy. *Physical Review B*, **2014**, 89,	3.3	44
114	Exact ab initio transport coefficients in bcc FeX (X=Cr, Cu, Mn, Ni, P, Si) dilute alloys. *Physical Review B*, **2014**, 90,	3.3	122
113	Recent radiation damage studies and developments of the Marlowe code. *Radiation Effects and Defects in Solids*, **2014**, 169, 592-602	0.9	13
112	Quantitative phase field model for dislocation sink strength calculations. *Computational Materials Science*, **2014**, 88, 50-60	3.2	27
111	Vacancy migration energy dependence on local chemical environment in FeCr alloys: A Density Functional Theory study. *Journal of Nuclear Materials*, **2014**, 452, 425-433	3.3	15
110	Kinetics of secondary phase precipitation during spinodal decomposition in duplex stainless steels: A kinetic Monte Carlo model Comparison with atom probe tomography experiments. *Journal of Nuclear Materials*, **2014**, 451, 361-365	3.3	21
109	Sintering of ferritic and austenitic nanopowders using Spark Plasma Sintering. *Metallurgical Research and Technology*, **2014**, 111, 305-310	0.9	2
108	Modeling of the self trapping of helium and the trap mutation in tungsten using DFT and empirical potentials based on DFT. *Journal of Materials Research*, **2014**, 29, 2374-2386	2.5	28
107	Influence of shape anisotropy of self-interstitials on dislocation sink efficiencies in Zr: Multiscale modeling. *Physical Review B*, **2014**, 90,	3.3	15
106	Atomistic modeling of carbon Cottrell atmospheres in bcc iron. *Journal of Physics Condensed Matter* , **2013**, 25, 025401	1.8	23
105	A brief summary of the progress on the EFDA tungsten materials program. *Journal of Nuclear Materials*, **2013**, 442, S173-S180	3.3	63

104	Sink strength calculations of dislocations and loops using OKMC. *Journal of Nuclear Materials*, **2013**, 442, 218-226	3.3	23
103	TEM investigations of the oxide layers formed on a 316L alloy in simulated PWR environment. *Journal of Materials Science*, **2013**, 48, 2861-2871	4.3	37
102	Spatial effects in the 800keV 3He implantation in W followed by isochronal annealing at 900K. *Nuclear Instruments & Methods in Physics Research B*, **2013**, 303, 87-90	1.2	4
101	Mechanisms of radiation strengthening in FeCr alloys as revealed by atomistic studies. *Journal of Nuclear Materials*, **2013**, 442, 470-485	3.3	30
100	Effect of the applied stress and the friction stress on the dislocation dissociation in face centered cubic metals. *Materials Letters*, **2013**, 97, 93-96	3.3	17
99	Self-interstitial defects in hexagonal close packed metals revisited: Evidence for low-symmetry configurations in Ti, Zr, and Hf. *Physical Review B*, **2013**, 87,	3.3	49
98	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. *Journal of Nuclear Materials*, **2013**, 432, 482-500	3.3	494
97	First principle-based AKMC modelling of the formation and medium-term evolution of point defect and solute-rich clusters in a neutron irradiated complex FeCuMnNiSiP alloy representative of reactor pressure vessel steels. *Journal of Nuclear Materials*, **2013**, 440, 143-152	3.3	30
96	Formation and evolution of MnNi clusters in neutron irradiated dilute Fe alloys modelled by a first principle-based AKMC method. *Journal of Nuclear Materials*, **2012**, 426, 198-207	3.3	66
95	First-principles molecular dynamics simulations of uranyl ion interaction at the water/rutile TiO2(110) interface. *Surface Science*, **2012**, 606, 1135-1141	1.8	13
94	Solute point defect interactions in bcc systems: Focus on first principles modelling in W and RPV steels. *Current Opinion in Solid State and Materials Science*, **2012**, 16, 115-125	12	75
93	Uranyl ion interaction at the water/NiO(100) interface: a predictive investigation by first-principles molecular dynamic simulations. *Journal of Chemical Physics*, **2012**, 137, 164701	3.9	4
92	Structure of nanoscale copper precipitates in neutron-irradiated Fe-Cu-C alloys. *Physical Review B*, **2012**, 85,	3.3	16
91	Review on the EFDA programme on tungsten materials technology and science. *Journal of Nuclear Materials*, **2011**, 417, 463-467	3.3	139
90	On the correlation between primary damage and long-term nanostructural evolution in iron under irradiation. *Journal of Nuclear Materials*, **2011**, 419, 122-133	3.3	27
89	Comparison of atomistic and elasticity approaches for carbon diffusion near line defects in iron. *Acta Materialia*, **2011**, 59, 6963-6974	8.4	41
88	Further development of large-scale atomistic modelling techniques for FeCr alloys. *Journal of Nuclear Materials*, **2011**, 409, 167-175	3.3	15
87	Modeling Microstructure and Irradiation Effects. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2011**, 42, 852-870	2.3	49

86	Kinetic study of phase transformation in a highly concentrated Fe□Cr alloy: Monte Carlo simulation versus experiments. *Acta Materialia*, **2011**, 59, 2404-2411	8.4	56
85	Investigation of hydrogen bonds and temperature effects on the water monolayer adsorption on rutile TiO2 (110) by first-principles molecular dynamics simulations. *Surface Science*, **2011**, 605, 1275-1280	1.8	23
84	Ab initio study of solute transition-metal interactions with point defects in bcc Fe. *Physical Review B* , **2010**, 81,	3.3	173
83	Interaction of a 12<111> screw dislocation with Cr precipitates in bcc Fe studied by molecular dynamics. *Physical Review B*, **2010**, 81,	3.3	41
82	Effect of the stress field of an edge dislocation on carbon diffusion in □ron: Coupling molecular statics and atomistic kinetic Monte Carlo. *Physical Review B*, **2010**, 82,	3.3	37
81	Comparison of empirical interatomic potentials for iron applied to radiation damage studies. *Journal of Nuclear Materials*, **2010**, 406, 19-38	3.3	179
80	Microstructure evolution of irradiated tungsten: Crystal effects in He and H implantation as modelled in the Binary Collision Approximation. *Journal of Nuclear Materials*, **2010**, 403, 89-100	3.3	34
79	Overview of the RPV-2 and INTERN-1 packages: From primary damage to microplasticity. *Journal of Nuclear Materials*, **2010**, 406, 175-186	3.3	20
78	Ab initio calculations and interatomic potentials for iron and iron alloys: Achievements within the Perfect Project. *Journal of Nuclear Materials*, **2010**, 406, 7-18	3.3	67
77	Atomistic Kinetic Monte Carlo studies of microchemical evolutions driven by diffusion processes under irradiation. *Journal of Nuclear Materials*, **2010**, 406, 55-67	3.3	57
76	Modeling the long-term evolution of the primary damage in ferritic alloys using coarse-grained methods. *Journal of Nuclear Materials*, **2010**, 406, 39-54	3.3	61
75	Microstructural evolution of irradiated tungsten: Ab initio parameterisation of an OKMC model. *Journal of Nuclear Materials*, **2010**, 403, 75-88	3.3	146
74	Isochronal annealing of electron-irradiated dilute Fe alloys modelled by an ab initio based AKMC method: Influence of solute□interstitial cluster properties. *Journal of Nuclear Materials*, **2010**, 407, 16-28	3.3	22
73	Introducing chemistry in atomistic kinetic Monte Carlo simulations of Fe alloys under irradiation. *Physica Status Solidi (B): Basic Research*, **2010**, 247, 9-22	1.3	40
72	Short- and long-range orders in Fe□Cr: A Monte Carlo study. *Journal of Applied Physics*, **2009**, 106, 104906	2.5	27
71	An object Kinetic Monte Carlo Simulation of the dynamics of helium and point defects in tungsten. *Journal of Nuclear Materials*, **2009**, 385, 223-227	3.3	147
70	A density functional theory assessment of the clustering behaviour of He and H in tungsten. *Journal of Nuclear Materials*, **2009**, 386-388, 109-111	3.3	117
69	Atomic and dislocation dynamics simulations of plastic deformation in reactor pressure vessel steel. *Journal of Nuclear Materials*, **2009**, 394, 174-181	3.3	11

68	Ferromagnetic compounds for high efficiency photovoltaic conversion: the case of AlP:Cr. *Physical Review Letters*, **2009**, 102, 227204	7.4	43
67	Molecular dynamics simulations of damage and plasticity: The role of ab initio calculations in the development of interatomic potentials. *Philosophical Magazine*, **2009**, 89, 3215-3234	1.6	4
66	Towards improved photovoltaic conversion using dilute magnetic semiconductors (abstract only). *Journal of Physics Condensed Matter*, **2008**, 20, 064226	1.8	4
65	Theoretical investigation of the uranyl ion sorption on the rutile TiO2(110) face. *Inorganic Chemistry* , **2008**, 47, 10991-7	5.1	30
64	Density functional calculations on structural materials for nuclear energy applications and functional materials for photovoltaic energy applications (abstract only). *Journal of Physics Condensed Matter*, **2008**, 20, 064224	1.8	
63	Self-trapped interstitial-type defects in iron. *Physical Review Letters*, **2008**, 100, 145503	7.4	84
62	Relevancy of displacement cascades features to the long term point defect cluster growth. *Journal of Nuclear Materials*, **2008**, 382, 103-111	3.3	16
61	Uranyl interaction with the hydrated (1 1 1) nickel face: A periodic density functional theory investigation. *Surface Science*, **2008**, 602, 3331-3337	1.8	8
60	Precipitation of the FeCu system: A critical review of atomic kinetic Monte Carlo simulations. *Journal of Nuclear Materials*, **2008**, 373, 387-401	3.3	80
59	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. *Journal of Nuclear Materials*, **2008**, 382, 154-159	3.3	50
58	Mean field rate theory and object kinetic Monte Carlo: A comparison of kinetic models. *Journal of Nuclear Materials*, **2008**, 382, 77-90	3.3	112
57	Ab initio study of Cr interactions with point defects in bcc Fe. *Physical Review B*, **2007**, 75,	3.3	239
56	Combined investigation of water sorption on TiO2 rutile (1 1 0) single crystal face: XPS vs. periodic DFT. *Surface Science*, **2007**, 601, 518-527	1.8	137
55	Stability and mobility of small vacancy and copper-vacancy clusters in bcc-Fe: An atomistic kinetic Monte Carlo study. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 255, 47-51	1.2	31
54	Ab initio calculations about intrinsic point defects and He in W. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 255, 23-26	1.2	178
53	Atomic kinetic Monte Carlo model based on ab initio data: Simulation of microstructural evolution under irradiation of dilute FeCuNiMnSi alloys. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 255, 78-84	1.2	47
52	Object kinetic Monte Carlo study of sink strengths. *Journal of Nuclear Materials*, **2007**, 360, 159-169	3.3	62
51	Structural investigation and electronic properties of the nickel ferrite NiFe2O4: a periodic density functional theory approach. *Journal of Physics Condensed Matter*, **2007**, 19, 346219	1.8	67

50	Density functional theory analysis of the structural and electronic properties of TiO2 rutile and anatase polytypes: performances of different exchange-correlation functionals. *Journal of Chemical Physics*, **2007**, 126, 154703	3.9	276
49	Optimisation of accurate rutile TiO2 (110), (100), (101) and (001) surface models from periodic DFT calculations. *Theoretical Chemistry Accounts*, **2007**, 117, 565-574	1.9	179
48	Atomistic modeling of an Fe system with a small concentration of C. *Computational Materials Science*, **2007**, 40, 119-129	3.2	148
47	Modelling of Radiation Damage in Fe-Cr Alloys. *Journal of ASTM International*, **2007**, 4, 100692		20
46	Theoretical first step towards an understanding of the uranyl ion sorption on the rutile TiO2(110) face: A DFT periodic and cluster study. *Radiochimica Acta*, **2006**, 94, 601-607	1.9	18
45	Migration energy of He in W revisited by ab initio calculations. *Physical Review Letters*, **2006**, 97, 196402	7.4	241
44	Periodic density functional theory investigation of the uranyl ion sorption on the TiO2 rutile (110) face. *Inorganic Chemistry*, **2006**, 45, 6568-70	5.1	28
43	Vacancy-solute complexes and their clusters in iron. *Applied Surface Science*, **2006**, 252, 3303-3308	6.7	28
42	Solute interaction with point defects in α-Fe during thermal ageing: A combined ab initio and atomic kinetic Monte Carlo approach. *Journal of Nuclear Materials*, **2006**, 351, 88-99	3.3	84
41	Effect of displacement cascade structure and defect mobility on the growth of point defect clusters under irradiation. *Journal of Nuclear Materials*, **2006**, 351, 39-46	3.3	31
40	Ab initio modelling of defect properties with substitutional and interstitials elements in steels and Zr alloys. *Journal of Nuclear Materials*, **2006**, 351, 1-19	3.3	86
39	Helium–self-interstitial atom interaction in α-iron. *Journal of Nuclear Materials*, **2006**, 351, 119-132	3.3	59
38	Dependence of radiation damage accumulation in iron on underlying models of displacement cascades and subsequent defect migration. *Journal of Nuclear Materials*, **2006**, 355, 89-103	3.3	43
37	Ab initio calculations of self-interstitial interaction and migration with solute atoms in bcc Fe. *Journal of Nuclear Materials*, **2006**, 359, 227-237	3.3	61
36	Fe-doped CuInSe2: An ab initio study of magnetic defects in a photovoltaic material. *Physical Review B*, **2005**, 71,	3.3	25
35	Ab initio atomic-scale modelling of iodine effects on hcp zirconium. *Philosophical Magazine*, **2005**, 85, 589-595	1.6	12
34	Ab initio calculations of some atomic and point defect interactions involving C and N in Fe. *Philosophical Magazine*, **2005**, 85, 533-540	1.6	18
33	Comparison of algorithms for multiscale modelling of radiation damage in Fe–Cu alloys. *Philosophical Magazine*, **2005**, 85, 417-428	1.6	9

32	Comparison between three complementary approaches to simulate large fluence irradiation: application to electron irradiation of thin foils. *Philosophical Magazine*, **2005**, 85, 541-547	1.6	27
31	Simulation of screw dislocation motion in iron by molecular dynamics simulations. *Physical Review Letters*, **2005**, 95, 215506	7.4	183
30	Two-band modeling of prime phase formation in Fe-Cr. *Physical Review B*, **2005**, 72,	3.3	175
29	Diffusion of phosphorus in Fe: An ab initio study. *Physical Review B*, **2005**, 71,	3.3	74
28	Ab initio atomic-scale determination of point-defect structure in hcp zirconium. *Philosophical Magazine*, **2005**, 85, 569-575	1.6	68
27	Interactions between dislocations and irradiation-induced defects in light water reactor pressure vessel steels. *Journal of Nuclear Materials*, **2005**, 346, 79-97	3.3	28
26	The influence of the internal displacement cascades structure on the growth of point defect clusters in radiation environment. *Nuclear Instruments & Methods in Physics Research B*, **2005**, 228, 181-186	1.2	12
25	Ab initio calculations of vacancy interactions with solute atoms in bcc Fe. *Nuclear Instruments & Methods in Physics Research B*, **2005**, 228, 137-141	1.2	60
24	Ab initio investigation of potential indium and gallium free chalcopyrite compounds for photovoltaic application. *Journal of Physics and Chemistry of Solids*, **2005**, 66, 2019-2023	3.9	75
23	Simulation of radiation damage in Fe alloys: an object kinetic Monte Carlo approach. *Journal of Nuclear Materials*, **2004**, 335, 121-145	3.3	243
22	Atomic-scale ab initio study of the ZrH system: II. Interaction of H with plane defects and mechanical properties. *Acta Materialia*, **2004**, 52, 1495-1502	8.4	74
21	Ab initio study of foreign interstitial atom (C, N) interactions with intrinsic point defects in Fe. *Physical Review B*, **2004**, 69,	3.3	312
20	Investigation of Glide Properties in Hexagonal Titanium and Zirconium: An Ab Initio Atomic Scale Study. *Solid Mechanics and Its Applications*, **2004**, 411-420	0.4	5
19	Formation Energies of Point Defects in Copper Indium Diselenide Using ab initio Methods. *Materials Research Society Symposia Proceedings*, **2003**, 763, 8101		1
18	Ab initio contribution to the study of complexes formed during dilute FeCu alloys radiation. *Nuclear Instruments & Methods in Physics Research B*, **2003**, 202, 44-50	1.2	62
17	Copper precipitation in iron: a comparison between metropolis Monte Carlo and lattice kinetic Monte Carlo methods. *Nuclear Instruments & Methods in Physics Research B*, **2003**, 202, 68-75	1.2	13
16	Ab initio calculation of intrinsic point defects in CuInSe2. *Journal of Physics and Chemistry of Solids*, **2003**, 64, 1657-1663	3.9	46
15	Atomic-scale Ab-initio study of the Zr-H system: I. Bulk properties. *Acta Materialia*, **2002**, 50, 3513-3526	8.4	133

14	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
13	Simulation of Irradiation Effects in Reactor Pressure Vessel Steels: the Reactor for Virtual Experiments (REVE) Project. *Journal of Testing and Evaluation*, **2002**, 30, 37	1	26
12	The role of Cu in displacement cascades examined by molecular dynamics. *Journal of Nuclear Materials*, **2001**, 294, 274-287	3.3	46
11	Atomic displacement cascade distributions in iron. *Journal of Nuclear Materials*, **2001**, 295, 179-188	3.3	42
10	Ab initio calculations of defects in Fe and dilute Fe-Cu alloys. *Physical Review B*, **2001**, 65,	3.3	346
9	Molecular Dynamics simulations of displacement cascades: role of the interatomic potentials and of the potential hardening. *Materials Research Society Symposia Proceedings*, **2000**, 650, 3241		1
8	Influence of the interatomic potentials on molecular dynamics simulations of displacement cascades. *Journal of Nuclear Materials*, **2000**, 280, 73-85	3.3	114
7	Kinetic Monte Carlo simulations of cascades in Fe alloys. *Materials Research Society Symposia Proceedings*, **2000**, 650, 3251		7
6	Simulation of the irradiation effects in reactor materials : The REVE project. *European Physical Journal Special Topics*, **2000**, 10, Pr6-191-Pr6-196		2
5	Kinetic Monte Carlo Simulations of Fecu Alloys. *Materials Research Society Symposia Proceedings*, **1998**, 538, 217		6
4	Kinetic Monte Carlo Simulations of FeCu Alloys. *Materials Research Society Symposia Proceedings*, **1998**, 540, 643		23
3	Computer simulations study of iron–copper alloy. *Radiation Effects and Defects in Solids*, **1997**, 141, 325-336	0.9	5
2	Massively parallel molecular dynamics simulations with EAM potentials. *Radiation Effects and Defects in Solids*, **1997**, 142, 9-21	0.9	38
1	The topological skeleton of cellular automaton dynamics. *Physica D: Nonlinear Phenomena*, **1997**, 103, 155-168	3.3	10