Christophe Domain

List of Publications by Year
in descending order

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180 papers	9,762 citations	34016 52 h-index	39575 94 g-index
181 all docs	181 docs citations	181 times ranked	5132 citing authors

#	Article	IF	Citations
1	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. Journal of Nuclear Materials, 2013, 432, 482-500.	1.3	610
2	Ab initiocalculations of defects in Fe and dilute Fe-Cu alloys. Physical Review B, 2001, 65, .	1.1	376
3	Ab initiostudy of foreign interstitial atom (C, N) interactions with intrinsic point defects inÎ±-Fe. Physical Review B, 2004, 69, .	1.1	351
4	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.	1.2	307
5	Migration Energy of He in W Revisited byAbÂInitioCalculations. Physical Review Letters, 2006, 97, 196402.	2.9	283
6	Simulation of radiation damage in Fe alloys: an object kinetic Monte Carlo approach. Journal of Nuclear Materials, 2004, 335, 121-145.	1.3	276
7	Ab initiostudy of Cr interactions with point defects in bcc Fe. Physical Review B, 2007, 75, .	1.1	269
8	Comparison of empirical interatomic potentials for iron applied to radiation damage studies. Journal of Nuclear Materials, 2010, 406, 19-38.	1.3	217
9	Optimisation of accurate rutile TiO2 (110), (100), (101) and (001) surface models from periodic DFT calculations. Theoretical Chemistry Accounts, 2007, 117, 565-574.	0.5	213
10	Simulation of Screw Dislocation Motion in Iron by Molecular Dynamics Simulations. Physical Review Letters, 2005, 95, 215506.	2.9	203
11	Ab initio calculations about intrinsic point defects and He in W. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 23-26.	0.6	197
12	Ab initiostudy of solute transition-metal interactions with point defects in bcc Fe. Physical Review B, 2010, 81, .	1.1	191
13	Two-band modeling ofÎ±-prime phase formation in Fe-Cr. Physical Review B, 2005, 72, .	1.1	189
14	Microstructural evolution of irradiated tungsten: Ab initio parameterisation of an OKMC model. Journal of Nuclear Materials, 2010, 403, 75-88.	1.3	177
15	Atomistic modeling of an Fe system with a small concentration of C. Computational Materials Science, 2007, 40, 119-129.	1.4	165
16	An object Kinetic Monte Carlo Simulation of the dynamics of helium and point defects in tungsten. Journal of Nuclear Materials, 2009, 385, 223-227.	1.3	157
17	Review on the EFDA programme on tungsten materials technology and science. Journal of Nuclear Materials, 2011, 417, 463-467.	1.3	157
18	Atomic-scale Ab-initio study of the Zr-H system: I. Bulk properties. Acta Materialia, 2002, 50, 3513-3526.	3.8	156

#	Article	IF	Citations
19	Combined investigation of water sorption on TiO2 rutile (110) single crystal face: XPS vs. periodic DFT. Surface Science, 2007, 601, 518-527. Exactab initiotransport coefficients in bcc<mml:math	0.8	150
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37	Object kinetic Monte Carlo study of sink strengths. Journal of Nuclear Materials, 2007, 360, 159-169.	1.3	72
38	Ab initio calculations and interatomic potentials for iron and iron alloys: Achievements within the Perfect Project. Journal of Nuclear Materials, 2010, 406, 7-18.	1.3	72
39	Ab initio calculations of self-interstitial interaction and migration with solute atoms in bcc Fe. Journal of Nuclear Materials, 2006, 359, 227-237.	1.3	69
40	A brief summary of the progress on the EFDA tungsten materials program. Journal of Nuclear Materials, 2013, 442, S173-S180.	1.3	69
41	Ab initio threshold displacement energies in iron. Materials Research Letters, 2016, 4, 219-225.	4.1	68
42	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.	0.6	67
43	Ab initio calculations of vacancy interactions with solute atoms in bcc Fe. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 137-141.	0.6	66
44	Self-interstitial defects in hexagonal close packed metals revisited: Evidence for low-symmetry configurations in Ti, Zr, and Hf. Physical Review B, 2013, 87, .	1.1	66
45	Atomistic Kinetic Monte Carlo studies of microchemical evolutions driven by diffusion processes under irradiation. Journal of Nuclear Materials, 2010, 406, 55-67.	1.3	65
46	Modeling the long-term evolution of the primary damage in ferritic alloys using coarse-grained methods. Journal of Nuclear Materials, 2010, 406, 39-54.	1.3	65
47	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.	1.3	65
48	Heliumâ€“self-interstitial atom interaction in Î±-iron. Journal of Nuclear Materials, 2006, 351, 119-132.	1.3	64
49	Kinetic study of phase transformation in a highly concentrated Feâ€“Cr alloy: Monte Carlo simulation versus experiments. Acta Materialia, 2011, 59, 2404-2411.	3.8	63
50	Non-equilibrium properties of interatomic potentials in cascade simulations in tungsten. Journal of Nuclear Materials, 2016, 470, 119-127.	1.3	63
51	First-principles study of point defects in an fcc Fe-10Ni-20Cr model alloy. Physical Review B, 2014, 89, .	1.1	61
52	Modeling Microstructure and Irradiation Effects. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2011, 42, 852-870.	1.1	54
53	Ab initio calculation of intrinsic point defects in CuInSe2. Journal of Physics and Chemistry of Solids, 2003, 64, 1657-1663.	1.9	52
54	Microstructural evolution under high flux irradiation of dilute Feâ€“CuNiMnSi alloys studied by an atomic kinetic Monte Carlo model accounting for both vacancies and self interstitials. Journal of Nuclear Materials, 2008, 382, 154-159.	1.3	52

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55	TEM investigations of the oxide layers formed on a 316L alloy in simulated PWR environment. Journal of Materials Science, 2013, 48, 2861-2871.	1.7	50
56	Atomic kinetic Monte Carlo model based on ab initio data: Simulation of microstructural evolution under irradiation of dilute Feâ€“CuNiMnSi alloys. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 78-84.	0.6	49
57	Comparison of atomistic and elasticity approaches for carbon diffusion near line defects in Î±-iron. Acta Materialia, 2011, 59, 6963-6974.	3.8	49
58	Ferromagnetic Compounds for High Efficiency Photovoltaic Conversion: The Case of AlP:Cr. Physical Review Letters, 2009, 102, 227204.	2.9	48
59	Organic thermoelectric devices based on a stable n-type nanocomposite printed on paper. Sustainable Energy and Fuels, 2018, 2, 199-208.	2.5	48
60	The role of Cu in displacement cascades examined by molecular dynamics. Journal of Nuclear Materials, 2001, 294, 274-287.	1.3	47
61	Introducing chemistry in atomistic kinetic Monte Carlo simulations of Fe alloys under irradiation. Physica Status Solidi (B): Basic Research, 2010, 247, 9-22.	0.7	46
62	Massively parallel molecular dynamics simulations with EAM potentials. Radiation Effects and Defects in Solids, 1997, 142, 9-21.	0.4	45
63	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.	1.3	45
64	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.	1.3	44
65	Interaction of a12âŸ¨111âŸ©screw dislocation with Cr precipitates in bcc Fe studied by molecular dynamics. Physical Review B, 2010, 81, .	1.1	44
66	Mechanisms of radiation strengthening in Feâ€“Cr alloys as revealed by atomistic studies. Journal of Nuclear Materials, 2013, 442, 470-485.	1.3	44
67	Atomic displacement cascade distributions in iron. Journal of Nuclear Materials, 2001, 295, 179-188.	1.3	42
68	Effect of the stress field of an edge dislocation on carbon diffusion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-iron: Coupling molecular statics and atomistic kinetic Monte Carlo. Physical Review B, 2010, 82, .	1.1	42
69	Multiscale modelling of the interaction of hydrogen with interstitial defects and dislocations in BCC tungsten. Nuclear Fusion, 2018, 58, 016006.	1.6	40
70	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.	1.3	36
71	Interactions between dislocations and irradiation-induced defects in light water reactor pressure vessel steels. Journal of Nuclear Materials, 2005, 346, 79-97.	1.3	35
72	Theoretical Investigation of the Uranyl Ion Sorption on the Rutile TiO₂(110) Face. Inorganic Chemistry, 2008, 47, 10991-10997.	1.9	35

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73	Atomistic modeling of carbon Cottrell atmospheres in bcc iron. Journal of Physics Condensed Matter, 2013, 25, 025401.	0.7	35
74	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.	1.2	35
75	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.	0.6	34
76	Solute â€“ ã€ˆ111ã€‰ interstitial loop interaction in Î±-Fe: A DFT study. Journal of Nuclear Materials, 2018, 499, 582-594.	1.3	34
77	First principle-based AKMC modelling of the formation and medium-term evolution of point defect and solute-rich clusters in a neutron irradiated complex Feâ€“CuMnNiSiP alloy representative of reactor pressure vessel steels. Journal of Nuclear Materials, 2013, 440, 143-152.	1.3	33
78	Vacancy-solute complexes and their clusters in iron. Applied Surface Science, 2006, 252, 3303-3308.	3.1	32
79	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.	1.3	32
80	Quantitative phase field model for dislocation sink strength calculations. Computational Materials Science, 2014, 88, 50-60.	1.4	31
81	Comparison between three complementary approaches to simulate â€˜â€‰largeâ€‰â€™ fluence irradiation: application to electron irradiation of thin foils. Philosophical Magazine, 2005, 85, 541-547.	0.7	30
82	A new scenario for â€¹câ€º vacancy loop formation in zirconium based on atomic-scale modeling. Acta Materialia, 2019, 179, 93-106.	3.8	30
83	Periodic Density Functional Theory Investigation of the Uranyl Ion Sorption on the TiO2Rutile (110) Face. Inorganic Chemistry, 2006, 45, 6568-6570.	1.9	29
84	Fe-dopedCuInSe2: Anab initiostudy of magnetic defects in a photovoltaic material. Physical Review B, 2005, 71, .	1.1	28
85	On the correlation between primary damage and long-term nanostructural evolution in iron under irradiation. Journal of Nuclear Materials, 2011, 419, 122-133.	1.3	28
86	Short- and long-range orders in Feâ€“Cr: A Monte Carlo study. Journal of Applied Physics, 2009, 106, .	1.1	27
87	Kinetics of secondary phase precipitation during spinodal decomposition in duplex stainless steels: A kinetic Monte Carlo model â€“ Comparison with atom probe tomography experiments. Journal of Nuclear Materials, 2014, 451, 361-365.	1.3	27
88	Improved atomistic Monte Carlo models based on ab-initio -trained neural networks: Application to FeCu and FeCr alloys. Physical Review B, 2017, 95, .	1.1	27
89	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.	1.4	27
90	Simulation of Irradiation Effects in Reactor Pressure Vessel Steels: the Reactor for Virtual Experiments (REVE) Project. Journal of Testing and Evaluation, 2002, 30, 37-46.	0.4	27

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91	Sink strength calculations of dislocations and loops using OKMC. Journal of Nuclear Materials, 2013, 442, 218-226.	1.3	25
92	Flexible thermoelectric device based on TiS2(HA)x n-type nanocomposite printed on paper. Organic Electronics, 2019, 68, 256-263.	1.4	25
93	Kinetic Monte Carlo Simulations of Fecu Alloys. Materials Research Society Symposia Proceedings, 1998, 540, 643.	0.1	24
94	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.	0.8	24
95	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.	1.3	24
96	Elastic dipole tensors and relaxation volumes of point defects in concentrated random magnetic Fe-Cr alloys. Computational Materials Science, 2021, 194, 110435.	1.4	24
97	Isochronal annealing of electron-irradiated dilute Fe alloys modelled by an ab initio based AKMC method: Influence of soluteâ€“interstitial cluster properties. Journal of Nuclear Materials, 2010, 407, 16-28.	1.3	23
98	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.	1.4	23
99	Investigation of solute segregation behavior using a correlative EBSD/TKD/APT methodology in a 16MND5 weld. Journal of Nuclear Materials, 2019, 523, 434-443.	1.3	22
100	Overview of the RPV-2 and INTERN-1 packages: From primary damage to microplasticity. Journal of Nuclear Materials, 2010, 406, 175-186.	1.3	21
101	Effect of the applied stress and the friction stress on the dislocation dissociation in face centered cubic metals. Materials Letters, 2013, 97, 93-96.	1.3	21
102	Modelling of Radiation Damage in Fe-Cr Alloys. Journal of ASTM International, 2007, 4, 100692.	0.2	21
103	Interatomic potential to study the formation of NiCr clusters in high Cr ferritic steels. Journal of Nuclear Materials, 2017, 484, 42-50.	1.3	20
104	Influence of vacancy diffusional anisotropy: Understanding the growth of zirconium alloys under irradiation and their microstructure evolution. Acta Materialia, 2020, 195, 631-644.	3.8	20
105	Ab initio calculations of some atomic and point defect interactions involving C and N in Fe. Philosophical Magazine, 2005, 85, 533-540.	0.7	19
106	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.	0.5	19
107	Vacancy migration energy dependence on local chemical environment in Feâ€“Cr alloys: A Density Functional Theory study. Journal of Nuclear Materials, 2014, 452, 425-433.	1.3	19
108	The dominant mechanisms for the formation of solute-rich clusters in low-Cu steels under irradiation. Materials Today Energy, 2020, 17, 100472.	2.5	19

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109	Further development of large-scale atomistic modelling techniques for Feâ€“Cr alloys. Journal of Nuclear Materials, 2011, 409, 167-175.	1.3	18
110	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.	0.6	18
111	Introducing ab initio based neural networks for transition-rate prediction in kinetic Monte Carlo simulations. Physical Review B, 2017, 95, .	1.1	18
112	Structure of nanoscale copper precipitates in neutron-irradiated Fe-Cu-C alloys. Physical Review B, 2012, 85, .	1.1	17
113	Atomic structure of grain boundaries in iron modeled using the atomic density function. Physical Review B, 2014, 89, .	1.1	17
114	Molecular dynamics investigation of the interaction of an edge dislocation with Frank loops in Feâ€“Ni10â€“Cr20 alloy. Journal of Nuclear Materials, 2015, 465, 301-310.	1.3	17
115	Interaction of transmutation products with precipitates, dislocations and grain boundaries in neutron irradiated W. Materialia, 2022, 22, 101370.	1.3	17
116	Relevancy of displacement cascades features to the long term point defect cluster growth. Journal of Nuclear Materials, 2008, 382, 103-111.	1.3	16
117	Influence of shape anisotropy of self-interstitials on dislocation sink efficiencies in Zr: Multiscale modeling. Physical Review B, 2014, 90, .	1.1	16
118	Recent radiation damage studies and developments of the Marlowe code. Radiation Effects and Defects in Solids, 2014, 169, 592-602.	0.4	16
119	Primary damage in tungsten using the binary collision approximation, molecular dynamic simulations and the density functional theory. Physica Scripta, 2016, T167, 014018.	1.2	16
120	Anti-aging treatment of nuclear power plant steel. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2018, 735, 73-80.	2.6	16
121	The topological skeleton of cellular automaton dynamics. Physica D: Nonlinear Phenomena, 1997, 103, 155-168.	1.3	15
122	Hydrogen accumulation around dislocation loops and edge dislocations: from atomistic to mesoscopic scales in BCC tungsten. Physica Scripta, 2017, T170, 014073.	1.2	15
123	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.	0.6	14
124	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.	0.6	13
125	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.	0.6	13
126	Ab initio atomic-scale modelling of iodine effects on hcp zirconium. Philosophical Magazine, 2005, 85, 589-595.	0.7	13

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127	First-principles molecular dynamics simulations of uranyl ion interaction at the water/rutile TiO2(110) interface. Surface Science, 2012, 606, 1135-1141.	0.8	13
128	Atomic and dislocation dynamics simulations of plastic deformation in reactor pressure vessel steel. Journal of Nuclear Materials, 2009, 394, 174-181.	1.3	12
129	Density functional theory-based cluster expansion to simulate thermal annealing in FeCrW alloys. Philosophical Magazine, 2017, 97, 299-317.	0.7	11
130	Comparison of algorithms for multiscale modelling of radiation damage in Feâ€“Cu alloys. Philosophical Magazine, 2005, 85, 417-428.	0.7	10
131	Numerical evaluation of dislocation loop sink strengths: A phase-field approach. Nuclear Instruments & Methods in Physics Research B, 2015, 352, 31-35.	0.6	10
132	A model of defect cluster creation in fragmented cascades in metals based on morphological analysis. Journal of Physics Condensed Matter, 2018, 30, 405701.	0.7	10
133	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.	1.3	10
134	Modelling the primary damage in Fe and W: Influence of the short range interactions on the cascade properties: Part 1 â€“ Energy transfer. Journal of Nuclear Materials, 2021, 547, 152816.	1.3	10
135	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.	1.3	10
136	Solute-point defect interactions, coupled diffusion, and radiation-induced segregation in fcc nickel. Physical Review Materials, 2021, 5, .	0.9	9
137	Uranyl interaction with the hydrated (111) nickel face: A periodic density functional theory investigation. Surface Science, 2008, 602, 3331-3337.	0.8	8
138	Modelling the primary damage in Fe and W: influence of the short-range interactions on the cascade properties: Part 2 â€“ multivariate multiple linear regression analysis of displacement cascades. Journal of Nuclear Materials, 2021, 549, 152887.	1.3	8
139	Kinetic Monte Carlo simulations of cascades in Fe alloys. Materials Research Society Symposia Proceedings, 2000, 650, 3251.	0.1	7
140	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
141	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.	1.2	7
142	Kinetic Monte Carlo simulation of nanostructural evolution under postâ€irradiation annealing in dilute FeMnNi. Physica Status Solidi C: Current Topics in Solid State Physics, 2015, 12, 20-24.	0.8	7
143	Carbon diffusion in bulk hcp zirconium: A multi-scale approach. Journal of Nuclear Materials, 2016, 473, 61-67.	1.3	7
144	Kinetic Monte Carlo Simulations of Irradiation Effects. , 2020, , 754-778.		7

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145	Physical mechanisms and parameters for models of microstructure evolution under irradiation in Fe alloys â€“ Part I: Pure Fe. Nuclear Materials and Energy, 2021, 29, 101069.	0.6	7
146	Development of a plasticity-oriented interatomic potential for CrFeMnNi high entropy alloys. Computational Materials Science, 2022, 203, 111165.	1.4	7
147	Kinetic Monte Carlo Simulations of Fecu Alloys. Materials Research Society Symposia Proceedings, 1998, 538, 217.	0.1	6
148	Towards improved photovoltaic conversion using dilute magnetic semiconductors (abstract only). Journal of Physics Condensed Matter, 2008, 20, 064226.	0.7	6
149	Computer simulations study of ironâ€“copper alloy. Radiation Effects and Defects in Solids, 1997, 141, 325-336.	0.4	5
150	Effect of annealing treatment at 550ÂÂ°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.	1.3	5
151	Phase-field calculations of sink strength in Al, Ni, and Fe: A detailed study of elastic effects. Computational Materials Science, 2020, 183, 109905.	1.4	5
152	Investigation of Glide Properties in Hexagonal Titanium and Zirconium: An Ab Initio Atomic Scale Study. Solid Mechanics and Its Applications, 2004, , 411-420.	0.1	5
153	Simulation of the irradiation effects in reactor materials : The REVE project. European Physical Journal Special Topics, 2000, 10, Pr6-191-Pr6-196.	0.2	5
154	Molecular dynamics simulations of damage and plasticity: The role ofab initiocalculations in the development of interatomic potentials. Philosophical Magazine, 2009, 89, 3215-3234.	0.7	4
155	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.	0.6	4
156	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.	0.2	4
157	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, 2022, 225, 117531.	3.8	4
158	Molecular Dynamics simulations of displacement cascades: role of the interatomic potentials and of the potential hardening. Materials Research Society Symposia Proceedings, 2000, 650, 3241.	0.1	3
159	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.	0.6	3
160	Unexpected role of prefactors in defects diffusion: The case of vacancies in the 55Fe-28Ni-17Cr concentrated solid-solution alloys. Acta Materialia, 2022, 237, 118153.	3.8	3
161	Sintering of ferritic and austenitic nanopowders using Spark Plasma Sintering. Metallurgical Research and Technology, 2014, 111, 305-310.	0.4	2
162	Atomistic Kinetic Monte Carlo and Solute Effects. , 2018, , 1-20.		2

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163	Object Kinetic Monte Carlo (OKMC): A Coarse-Grained Approach to Radiation Damage. , 2018, , 1-26.		2
164	Atomistic Modeling of Radiation Damage in Metallic Alloys. , 2018, , 1-30.		2
165	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.	0.2	2
166	Interaction between interstitial carbon atoms and a Â½ â€©1â€‰1â€‰1â€ª 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.	0.7	2
167	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.	0.6	2
168	Atomistic investigation of elementary dislocation properties influencing mechanical behaviour of Cr15Fe46Mn17Ni22 alloy and Cr20Fe70Ni10 alloy. Computational Materials Science, 2022, 211, 111508.	1.4	2
169	Formation Energies of Point Defects in Copper Indium Diselenide Using ab initio Methods. Materials Research Society Symposia Proceedings, 2003, 763, 8101.	0.1	1
170	Study of solute segregation behavior at carbideâ€“ferrite interfaces in 16MND5 welds. Journal of Nuclear Materials, 2020, 542, 152531.	1.3	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.	0.7	1
172	Atomistic Modeling of Radiation Damage in Metallic Alloys. , 2019, , 673-701.		1
173	Ultrasonic wave propagation on parallel machines. , 1994, , .		0
174	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.	0.7	0
175	Multiscale Modelling of Microstructure Evolution under Radiation Damage of Steels Based on Atomistic to Mesoscale Methods. EPJ Web of Conferences, 2013, 51, 02004.	0.1	0
176	Atomic modelling of carbon atom diffusion in monoclinic zirconia volume, subsurface and surface. Journal of Nuclear Materials, 2020, 537, 152193.	1.3	0
177	Outils de simulation Ã l'Ã©chelle atomique pour traiter la chimie et la plasticitÃ©. , 2009, , .		0
178	Atomic kinetic Monte Carlo modeling of multi-component Fe dilute alloys under irradiation. , 2014, , .		0
179	Atomistic Kinetic Monte Carlo and Solute Effects. , 2020, , 2437-2456.		0
180	Object Kinetic Monte Carlo (OKMC): A Coarse-Grained Approach to Radiation Damage. , 2020, , 1287-1312.		0