Maria J Caturla

List of Publications by Year
in descending order

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135 papers	2,900 citations	109321 35 h-index	197818 49 g-index
138 all docs	138 docs citations	138 times ranked	2039 citing authors

#	Article	IF	Citations
1	Comparative study of radiation damage accumulation in Cu and Fe. Journal of Nuclear Materials, 2000, 276, 13-21.	2.7	204
2	Atomistic shock Hugoniot simulation of single-crystal copper. Journal of Applied Physics, 2004, 96, 3793-3799.	2.5	200
3	MMonCa: An Object Kinetic Monte Carlo simulator for damage irradiation evolution and defect diffusion. Computer Physics Communications, 2013, 184, 2703-2710.	7.5	100
4	He diffusion in irradiatedÎ±â^'Fe: Anab-initio-based rate theory model. Physical Review B, 2007, 75, .	3.2	99
5	Formation of a Metallic Contact: Jump to Contact Revisited. Physical Review Letters, 2007, 98, 206801.	7.8	73
6	The fraction of substitutional boron in silicon during ion implantation and thermal annealing. Applied Physics Letters, 1998, 72, 2736-2738.	3.3	71
7	Simulation of defect evolution in irradiated materials: Role of intracascade clustering and correlated recombination. Physical Review B, 2007, 75, .	3.2	71
8	Densification of fused silica due to shock waves and its implications for 351 nm laser induced damage. Optics Express, 2001, 8, 611.	3.4	70
9	The EU programme for modelling radiation effects in fusion reactor materials: An overview of recent advances and future goals. Journal of Nuclear Materials, 2009, 386-388, 1-7.	2.7	68
10	Modeling the long-term evolution of the primary damage in ferritic alloys using coarse-grained methods. Journal of Nuclear Materials, 2010, 406, 39-54.	2.7	65
11	Disordering and defect production in silicon by keV ion irradiation studied by molecular dynamics. Nuclear Instruments & Methods in Physics Research B, 1995, 106, 1-8.	1.4	61
12	Temperature-dependent defect properties from ion-irradiation in Pu(Ga). Journal of Alloys and Compounds, 2004, 368, 62-74.	5.5	60
13	Mechanical property degradation in irradiated materials: A multiscale modeling approach. Nuclear Instruments & Methods in Physics Research B, 2001, 180, 23-31.	1.4	59
14	Recrystallization of a planar amorphousâ€crystalline interface in silicon by low energy recoils: A molecular dynamics study. Journal of Applied Physics, 1995, 77, 3121-3125.	2.5	58
15	Formation energy of vacancies in FeCr alloys: Dependence on Cr concentration. Journal of Nuclear Materials, 2011, 408, 18-24.	2.7	54
16	Influence of the picosecond defect distribution on damage accumulation in irradiated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Fe. Physical Review B, 2012, 85, .	3.2	47
17	Surface effects and statistical laws of defects in primary radiation damage: Tungsten vs. iron. Europhysics Letters, 2016, 115, 36001.	2.0	46
18	Atomistic sliding mechanisms of the Î£=5 symmetric tilt grain boundary in bcc iron. Philosophical Magazine, 2005, 85, 3795-3807.	1.6	45

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19	Fundamental Studies of Plutonium Aging. MRS Bulletin, 2001, 26, 679-683.	3.5	43
20	Fused Silica Final Optics for Inertial Fusion Energy: Radiation Studies and System-Level Analysis. Fusion Science and Technology, 2003, 43, 540-558.	1.1	43
21	Multiscale modeling of radiation damage: applications to damage production by GeV proton irradiation of Cu and W, and pulsed irradiation effects in Cu and Fe. Journal of Nuclear Materials, 2001, 296, 90-100.	2.7	42
22	Large enhancement of boron solubility in silicon due to biaxial stress. Applied Physics Letters, 2002, 80, 4738-4740.	3.3	41
23	High-pressure, high-strain-rate lattice response of shocked materials. Physics of Plasmas, 2003, 10, 1569-1576.	1.9	41
24	Kinetic Monte Carlo simulations applied to irradiated materials: The effect of cascade damage in defect nucleation and growth. Journal of Nuclear Materials, 2006, 351, 78-87.	2.7	41
25	Modelling irradiation effects in fusion materials. Fusion Engineering and Design, 2007, 82, 2413-2421.	1.9	40
26	Influence of carbon on the kinetics of He migration and clustering in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>-Fe</mml:mtext></mml:mrow></mml:math>from first principles. Physical Review B, 2009, 80, .	3.2	40
27	Simulation of damage production and accumulation in vanadium. Journal of Nuclear Materials, 2000, 276, 221-229.	2.7	39
28	Differences in deformation processes in nanocrystalline nickel with low- and high-angle boundaries from atomistic simulations. Applied Physics Letters, 2004, 84, 598-600.	3.3	39
29	Defect production and annealing kinetics in elemental metals and semiconductors. Journal of Nuclear Materials, 1997, 251, 13-33.	2.7	38
30	Effects of elastic interactions on post-cascade radiation damage evolution in kinetic Monte Carlo simulations. Philosophical Magazine, 2005, 85, 661-675.	1.6	38
31	Surface-induced vacancy loops and damage dispersion in irradiated Fe thin films. Acta Materialia, 2015, 101, 22-30.	7.9	38
32	Modeling microstructure evolution of f.c.c. metals under irradiation in the presence of He. Journal of Nuclear Materials, 2003, 323, 163-168.	2.7	37
33	Mechanical Annealing of Metallic Electrodes at the Atomic Scale. Physical Review Letters, 2012, 108, 205502.	7.8	37
34	Perspectives on multiscale modelling and experiments to accelerate materials development for fusion. Journal of Nuclear Materials, 2021, 554, 153113.	2.7	37
35	Multiple film plane diagnostic for shocked lattice measurements (invited). Review of Scientific Instruments, 2003, 74, 1929-1934.	1.3	36
36	Atomic scale models of ion implantation and dopant diffusion in silicon. Thin Solid Films, 2000, 365, 219-230.	1.8	35

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37	Metals far from equilibrium: From shocks to radiation damage. Nuclear Instruments & Methods in Physics Research B, 2003, 202, 56-63.	1.4	32
38	Helium and point defect accumulation: (ii) kinetic modelling. Comptes Rendus Physique, 2008, 9, 401-408.	0.9	29
39	Effect of self-interstitial cluster migration on helium diffusion in iron. Journal of Nuclear Materials, 2007, 362, 141-145.	2.7	23
40	Theoretical study of the dynamics of atomic hydrogen adsorbed on graphene multilayers. Physical Review B, 2015, 91, .	3.2	23
41	Threshold energy of formation of an oxygen vacancy defect in SiO2 by atomic displacements using molecular dynamics. Fusion Engineering and Design, 2005, 75-79, 1027-1030.	1.9	22
42	Direct simulation of resistivity recovery experiments in carbon-doped Î±-iron. Physica Scripta, 2011, T145, 014049.	2.5	21
43	Cascade damage evolution: rate theory versus kinetic Monte Carlo simulations. Journal of Computer-Aided Materials Design, 2007, 14, 171-181.	0.7	20
44	Laser damage probability studies of fused silica modified by MeV ion implantation. Nuclear Instruments & Methods in Physics Research B, 2003, 207, 72-79.	1.4	18
45	Dynamic bonding of metallic nanocontacts: Insights from experiments and atomistic simulations. Physical Review B, 2016, 93, .	3.2	17
46	Defect production and damage evolution in Al: a molecular dynamics and Monte Carlo computer simulation. Nuclear Instruments & Methods in Physics Research B, 1999, 153, 105-115.	1.4	16
47	Abnormal stress drop at the yield point of aluminum nanowires: A molecular dynamics study. Physical Review B, 2011, 83, .	3.2	16
48	Study of cascades damage in Ni by MD with different interatomic potentials. Journal of Nuclear Materials, 2007, 367-370, 298-304.	2.7	15
49	Effect of ion flux on helium retention in helium-irradiated tungsten. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 81-83.	1.4	15
50	Influence of Relativistic Effects on the Contact Formation of Transition Metals. Physical Review Letters, 2018, 120, 076802.	7.8	15
51	The primary damage state and its evolution over multiple length and time scales: Recent atomic-scale computer simulation studies. Radiation Effects and Defects in Solids, 1999, 148, 95-126.	1.2	14
52	Atomistic simulations of threshold displacement energies in SiO2. Journal of Nuclear Materials, 2004, 329-333, 1190-1193.	2.7	14
53	Identification and characterization of defects produced in irradiated fused silica through molecular dynamics. Journal of Nuclear Materials, 2007, 367-370, 344-349.	2.7	13
54	Controlled rippling of graphene via irradiation and applied strain modify its mechanical properties: a nanoindentation simulation study. Physical Chemistry Chemical Physics, 2016, 18, 13897-13903.	2.8	13

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55	Insights from atomistic models on loop nucleation and growth in Î±-Fe thin films under Fe+ 100â€¯keV irradiation. Journal of Nuclear Materials, 2019, 521, 71-80.	2.7	13
56	Mechanical, Electrical, and Magnetic Properties of Ni Nanocontacts. IEEE Nanotechnology Magazine, 2008, 7, 165-168.	2.0	12
57	Molecular dynamics study of structure transformation and H effects in irradiated silica. Journal of Nuclear Materials, 2009, 386-388, 75-78.	2.7	12
58	Impurity effects on He diffusion in Î±-Fe. Journal of Nuclear Materials, 2009, 386-388, 33-35.	2.7	12
59	Permanent modifications in silica produced by ion-induced high electronic excitation: experiments and atomistic simulations. Scientific Reports, 2017, 7, 10641.	3.3	12
60	Role of first-neighbor geometry in the electronic and mechanical properties of atomic contacts. Physical Review B, 2018, 97, .	3.2	12
61	Multiscale modelling for fusion and fission materials: The M4F project. Nuclear Materials and Energy, 2021, 29, 101051.	1.3	12
62	Structural modifications in fused silica due to laser-damage-induced shock compression. , 2002, , .		11
63	Modeling defect production in silica glass due to energetic recoils using molecular dynamics simulations. Journal of Nuclear Materials, 2002, 307-311, 891-894.	2.7	11
64	Threats to ICF reactor materials: computational simulations of radiation damage induced topological changes in fused silica. Nuclear Instruments & Methods in Physics Research B, 2003, 202, 88-92.	1.4	11
65	Graphene flakes obtained by local electro-exfoliation of graphite with a STM tip. Physical Chemistry Chemical Physics, 2017, 19, 8061-8068.	2.8	11
66	Object Kinetic Monte Carlo calculations of irradiated Feâ€“Cr dilute alloys: The effect of the interaction radius between substitutional Cr and self-interstitial Fe. Nuclear Instruments & Methods in Physics Research B, 2011, 269, 1684-1688.	1.4	10
67	Advanced materials characterization and modeling using synchrotron, neutron, TEM, and novel micro-mechanical techniquesâ€”A European effort to accelerate fusion materials development. Journal of Nuclear Materials, 2013, 442, S834-S845.	2.7	10
68	Modeling contact formation between atomic-sized gold tips via molecular dynamics. Journal of Physics: Conference Series, 2015, 574, 012045.	0.4	10
69	Object kinetic Monte Carlo methods applied to modeling radiation effects in materials. Computational Materials Science, 2019, 156, 452-459.	3.0	10
70	Title is missing!. Journal of Computer-Aided Materials Design, 1998, 5, 243-264.	0.7	9
71	Annealing Kinetics of Single Displacement Cascades in Ni: An Atomic Scale Computer Simulation. Materials Research Society Symposia Proceedings, 1998, 540, 685.	0.1	9
72	Heavy ion irradiation and annealing of lead: atomistic simulations and experimental validation. Journal of Nuclear Materials, 2000, 276, 186-193.	2.7	9

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73	Temperature dependence of damage accumulation in Î±-zirconium. Journal of Nuclear Materials, 2007, 367-370, 338-343.	2.7	9
74	Molecular dynamics simulations of defect production in graphene by carbon irradiation. Nuclear Instruments & Methods in Physics Research B, 2015, 352, 225-228.	1.4	9
75	Influence of free surfaces on microstructure evolution of radiation damage in Fe from molecular dynamics and object kinetic Monte Carlo calculations. Physica Status Solidi (A) Applications and Materials Science, 2016, 213, 2969-2973.	1.8	9
76	Comparative study of damage accumulation in iron under magnetic and inertial fusion conditions. Journal of Nuclear Materials, 2000, 283-287, 768-772.	2.7	8
77	Correlating TEM images of damage in irradiated materials to molecular dynamics simulations. Journal of Nuclear Materials, 2002, 307-311, 988-992.	2.7	7
78	Kinetic Monte Carlo modelling of neutron irradiation damage in iron. Fusion Engineering and Design, 2007, 82, 2666-2670.	1.9	7
79	Influence of self-interstitial mobility on damage accumulation in zirconium under fission irradiation conditions. Journal of Nuclear Materials, 2007, 362, 293-299.	2.7	7
80	Stress-strain curves of aluminum nanowires: Fluctuations in the plastic regime and absence of hardening. Physical Review B, 2008, 78, .	3.2	7
81	Microstructure evolution of irradiated structural materials in nuclear power plants. , 2010, , 189-235.		7
82	An object kinetic Monte Carlo method to model precipitation and segregation in alloys under irradiation. Journal of Nuclear Materials, 2021, 557, 153236.	2.7	7
83	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.	1.3	7
84	Activation and damage of fusion materials and tritium effects in inertial fusion reactors: Strategy for adequate irradiation. Laser and Particle Beams, 2005, 23, .	1.0	6
85	Stability of vacancy clusters in FeCr alloys: A study of the Cr concentration dependence. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 46-50.	1.4	6
86	Some Issues in Liquid Metals Research. Metals, 2015, 5, 2128-2133.	2.3	6
87	Bulk atomic relocation in low-energy collision cascades in silicon: Molecular Dynamics versus Monte Carlo simulations. Nuclear Instruments & Methods in Physics Research B, 1994, 90, 363-368.	1.4	5
88	On the stressâ€strain curves in gold and aluminum nanowires. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 2119-2122.	0.8	5
89	Damage accumulation in pure iron and high concentrated Feâ€“12.5 at% Cr alloy: comparison between object kinetic Monte Carlo and cluster dynamics. Radiation Effects and Defects in Solids, 2014, 169, 185-193.	1.2	5
90	Microstructure Evolution in Fe and Fe-Cr Alloys with OKMC Methods. EPJ Web of Conferences, 2016, 115, 03001.	0.3	5

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91	Spin-lattice dynamics simulation of the Einsteinâ€“de Haas effect. Computational Materials Science, 2022, 209, 111359.	3.0	5
92	X-Ray Diffraction from Shocked Crystals: Experiments and Predictions of Molecular Dynamics Simulations. AIP Conference Proceedings, 2004, , .	0.4	4
93	The role of the fused silica stoichiometry on the intrinsic defects concentration. Journal of Nuclear Materials, 2007, 367-370, 1122-1127.	2.7	4
94	Defect energetics in Feâ€“Cr alloys from empirical interatomic potentials. Journal of Nuclear Materials, 2011, 417, 1050-1053.	2.7	4
95	Kinetic Monte Carlo Algorithms for Nuclear Materials Applications. , 2018, , 1-22.		4
96	Refined electron-spin transport model for single-element ferromagnetic systems: Application to nickel nanocontacts. Physical Review B, 2020, 102, .	3.2	4
97	Directional bonding explains the high conductance of atomic contacts in bcc metals. Physical Review B, 2020, 101, .	3.2	4
98	Collision cascade effects near an edge dislocation dipole in alpha-Fe: Induced dislocation mobility and enhanced defect clustering. Journal of Nuclear Materials, 2021, 543, 152459.	2.7	4
99	Surface Effects During Ion Beam Processing of Materials. Materials Research Society Symposia Proceedings, 1995, 396, 3.	0.1	3
100	Relative Stability of Silicon Self-Interstitial Defects. Materials Research Society Symposia Proceedings, 2000, 610, 11101.	0.1	3
101	Pulse frequency effect on neutron damage in Î±-Iron:A KMC analysis. Materials Research Society Symposia Proceedings, 2001, 677, 251.	0.1	3
102	Results from systematic modeling of neutron damage in inertial fusion energy reactors. Fusion Engineering and Design, 2002, 60, 55-63.	1.9	3
103	Time-Dependent Neutronics in Structural Materials of Inertial Fusion Reactors and Simulation of Defect Accumulation in Pulsed Fe and SiC. Fusion Science and Technology, 2003, 43, 384-392.	1.1	3
104	Long-term behaviour of irradiated hcp Zr using Monte Carlo simulations. Nuclear Instruments & Methods in Physics Research B, 2005, 228, 176-180.	1.4	3
105	Non-Gaussian tails in the probability distribution function of heat exchanged during isothermal stretching of aluminum and gold nanowires. Physical Review E, 2009, 80, 030105.	2.1	3
106	Object Kinetic Monte Carlo calculations of electron and He irradiation of nickel. Journal of Nuclear Materials, 2009, 386-388, 90-92.	2.7	3
107	Surface damage in TEM thick Î±-Fe samples by implantation with 150 keV Fe ions. Nuclear Instruments & Methods in Physics Research B, 2015, 352, 217-220.	1.4	3
108	Revealing the Geometry and Conductance of Double-Stranded Atomic Chains of Gold. Journal of Physical Chemistry C, 2020, 124, 26596-26602.	3.1	3

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109	Relocation cross-sections in silicon: Theoretical models. Nuclear Instruments & Methods in Physics Research B, 1995, 102, 19-23.	1.4	2
110	Molecular Dynamics Simulation of Cascade Damage in Gold. Materials Research Society Symposia Proceedings, 1996, 439, 367.	0.1	2
111	Dose Rate Effects During Damage Accumulation in Silicon. Materials Research Society Symposia Proceedings, 1996, 439, 125.	0.1	2
112	Linking ab initio Energetics to Experiment: Kinetic Monte Carlo Simulation of Transient Enhanced Diffusion of B in Si. Materials Research Society Symposia Proceedings, 1998, 538, 291.	0.1	2
113	Multiscale Modeling of Radiation Damage of Metals and SIC in Inertial Fusion Reactors. Fusion Science and Technology, 2001, 39, 579-584.	0.6	2
114	Multiscale modeling study of pulsed damage accumulation in Î±-Fe under inertial fusion conditions. Journal of Nuclear Materials, 2002, 307-311, 907-911.	2.7	2
115	Molecular Dynamics Simulations of Energy Deposition in Solids. Advances in Quantum Chemistry, 2004, 45, 79-98.	0.8	2
116	Radiation damage in metals, and amorphous silica in inertial fusion reactors: Modeling and experiments. European Physical Journal Special Topics, 2006, 133, 805-809.	0.2	2
117	Molecular dynamics simulations of irradiation of Î±-Fe thin films with energetic Fe ions under channeling conditions. Journal of Nuclear Materials, 2014, 452, 453-456.	2.7	2
118	Disrupted chimera ordering of magnetization within FeCl 2 layers. Europhysics Letters, 2018, 123, 60004.	2.0	2
119	Effect of cascade overlap and C15 clusters on the damage evolution in Fe: An OKMC study. Materialia, 2022, 21, 101344.	2.7	2
120	Insight into the materials choice for inertial fusion energy reactors considering radiation damage: Neutron irradiation intensities and basic knowledge from multiscale modeling. Laser and Particle Beams, 2002, 20, 627-631.	1.0	1
121	Defect diffusion in hcp Zirconium: A kinetic Monte Carlo approach. Materials Research Society Symposia Proceedings, 2003, 792, 178.	0.1	1
122	Mechanical and electrical properties of Ni nanocontacts. , 2006, , .		1
123	Molecular dynamics study of defect in amorphous silica; generation and migration. Journal of Physics: Conference Series, 2008, 112, 032032.	0.4	1
124	Defect production in Ar irradiated graphene membranes under different initial applied strains. Nuclear Instruments & Methods in Physics Research B, 2017, 393, 44-48.	1.4	1
125	Problems encountered in calculations of collisional mixing in compounds. Journal of Physics Condensed Matter, 1993, 5, A303-A304.	1.8	0
126	Depth profiling of isotopic markers. Vacuum, 1994, 45, 1123-1124.	3.5	0

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127	Depth resolution in depth profiling of marker layers by energetic ion bombardment. Nuclear Instruments & Methods in Physics Research B, 1995, 95, 91-96.	1.4	0
128	Modeling and Computer Simulation: Kinetic Monte Carlo/ Molecular Dynamics. , 2001, , 5697-5700.		0
129	Modeling of time-dependent damage in structural wall of inertial fusion reactors and new tight binding model for SiC. Fusion Engineering and Design, 2003, 69, 795-801.	1.9	0
130	Defect based spin mediation in Î´-phase plutonium. Materials Research Society Symposia Proceedings, 2003, 802, 227.	0.1	0
131	Advances in Materials Physics for IFE at DENIM. , 2007, , .		0
132	He production and induced swelling in KOYO-F. Journal of Physics: Conference Series, 2008, 112, 032042.	0.4	0
133	Influence of Self-Interstitial Mobility on He-Vacancy Cluster Nucleation and Growth in Nickel. Fusion Science and Technology, 2009, 56, 314-317.	1.1	0
134	Radiation effects across classes of materials. Physica Status Solidi (A) Applications and Materials Science, 2016, 213, 2959-2959.	1.8	0
135	Probability distribution for heat exchange in plastic deformation. Physical Review E, 2021, 104, 034101.	2.1	0