

# Blas P Uberuaga

## List of Publications by Year in descending order

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275  
papers

25,859  
citations

36203

51  
h-index

6818

155  
g-index

288  
all docs

288  
docs citations

288  
times ranked

22166  
citing authors

#	ARTICLE	IF	CITATIONS
1	A climbing image nudged elastic band method for finding saddle points and minimum energy paths. Journal of Chemical Physics, 2000, 113, 9901-9904.	1.2	15,067
2	Efficient Annealing of Radiation Damage Near Grain Boundaries via Interstitial Emission. Science, 2010, 327, 1631-1634.	6.0	884
3	Radiation-induced amorphization resistance and radiation tolerance in structurally related oxides. Nature Materials, 2007, 6, 217-223.	13.3	464
4	Defect-interface interactions. Progress in Materials Science, 2015, 74, 125-210.	16.0	450
5	Radiation damage tolerant nanomaterials. Materials Today, 2013, 16, 443-449.	8.3	423
6	Machine learning bandgaps of double perovskites. Scientific Reports, 2016, 6, 19375.	1.6	354
7	Band-gap engineering for removing shallow traps in rare-earth Lu $\text{AlO}_3$ thin films. Scientific Reports, 2017, 7, 11711.	1.1	288
8	Synchronization of trajectories in canonical molecular-dynamics simulations: Observation, explanation, and exploitation. Journal of Chemical Physics, 2004, 120, 6363-6374.	1.2	221
9	Defect Structure of Flash-Sintered Strontium Titanate. Journal of the American Ceramic Society, 2012, 95, 2531-2536.	1.9	148
10	Direct Transformation of Vacancy Voids to Stacking Fault Tetrahedra. Physical Review Letters, 2007, 99, 135501.	2.9	143
11	Cooperativity among defect sites in $\text{Al}_2\text{O}_3$ . Physical Review B, 2009, 79, 045411.	1.1	142
12	First-principles prediction of disordering tendencies in pyrochlore oxides. Physical Review B, 2009, 79, 045411.	1.1	140
13	Chapter 4 Accelerated Molecular Dynamics Methods: Introduction and Recent Developments. Annual Reports in Computational Chemistry, 2009, , 79-98.	0.9	139
14	The relationship between grain boundary structure, defect mobility and grain boundary sink efficiency. Scientific Reports, 2015, 5, 9095.	1.6	136
15	Vacancy-mediated dopant diffusion activation enthalpies for germanium. Applied Physics Letters, 2008, 92, 052105.	1.5	132
16	Comparison of screened hybrid density functional theory to diffusion Monte Carlo in calculations of total energies of silicon phases and defects. Physical Review B, 2006, 74, 045111.	1.1	131
17	U and Xe transport in $\text{UO}_2$ . Density functional theory calculations. Physical Review B, 2011, 84, 045111.	1.1	110
18	Competing Kinetics and He Bubble Morphology in W. Physical Review Letters, 2015, 114, 105502.	2.9	108

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19	Role of atomic structure on grain boundary-defect interactions in Cu. <i>Physical Review B</i> , 2012, 85, .	1.1	107
20	Stick-slip behavior of grain boundaries studied by accelerated molecular dynamics. <i>Physical Review B</i> , 2007, 75, .	1.1	98
21	Structure and Mobility of Defects Formed from Collision Cascades in MgO. <i>Physical Review Letters</i> , 2004, 92, 115505.	2.9	96
22	Anisotropic thermal conductivity in uranium dioxide. <i>Nature Communications</i> , 2014, 5, 4551.	5.8	93
23	Efficient <i>Ab Initio</i> Modeling of Random Multicomponent Alloys. <i>Physical Review Letters</i> , 2016, 116, 105501.	2.9	93
24	Role of Antisite Disorder on Preamorphization Swelling in Titanate Pyrochlores. <i>Physical Review Letters</i> , 2012, 108, 195504.	2.9	85
25	The parallel replica dynamics method “Coming of age”. <i>Computational Materials Science</i> , 2015, 100, 90-103.	1.4	85
26	First-principles calculations of uranium diffusion in uranium dioxide. <i>Physical Review B</i> , 2012, 86, .	1.1	83
27	Atomistic modeling of intrinsic and radiation-enhanced fission gas (Xe) diffusion in $^{238}\text{UO}_2$ . Implications for nuclear fuel performance modeling. <i>Journal of Nuclear Materials</i> , 2014, 451, 225-242.	1.3	83
28	Diffusion and defect reactions between donors, C, and vacancies in Ge. II. Atomistic calculations of related complexes. <i>Physical Review B</i> , 2008, 77, .	1.1	81
29	Dynamical simulations of radiation damage and defect mobility in MgO. <i>Physical Review B</i> , 2005, 71, .	1.1	79
30	Diffusion and transformation kinetics of small helium clusters in bulk tungsten. <i>Physical Review B</i> , 2014, 90, .	1.1	79
31	Diffusion of Ge below the Si(100) Surface: Theory and Experiment. <i>Physical Review Letters</i> , 2000, 84, 2441-2444.	2.9	78
32	Grain Boundaries in Uranium Dioxide: Scanning Electron Microscopy Experiments and Atomistic Simulations. <i>Journal of the American Ceramic Society</i> , 2011, 94, 1893-1900.	1.9	78
33	Radiation Tolerance of Nanocrystalline Ceramics: Insights from Yttria Stabilized Zirconia. <i>Scientific Reports</i> , 2015, 5, 7746.	1.6	77
34	Carbon, dopant, and vacancy interactions in germanium. <i>Journal of Applied Physics</i> , 2007, 102, 083707.	1.1	76
35	Vacancy-arsenic clusters in germanium. <i>Applied Physics Letters</i> , 2007, 91, .	1.5	75
36	Influence of interface sink strength on the reduction of radiation-induced defect concentrations and fluxes in materials with large interface area per unit volume. <i>Physical Review B</i> , 2011, 84, .	1.1	72

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37	Defect kinetics in spinels: Long-time simulations of MgAl <sub>2</sub> O <sub>4</sub> , MgGa <sub>2</sub> O <sub>4</sub> , and MgIn <sub>2</sub> O <sub>4</sub> . Physical Review B, 2007, 75, .	1.1	68
38	The Influence of Grain Boundaries on Radiation-Induced Point Defect Production in Materials: A Review of Atomistic Studies. Jom, 2013, 65, 360-373.	0.9	68
39	Chemical manipulation of hydrogen induced high p-type and n-type conductivity in Ga <sub>2</sub> O <sub>3</sub> . Scientific Reports, 2020, 10, 6134.	1.6	65
40	MgO addimer diffusion on MgO(100): A comparison of ab initio and empirical models. Physical Review B, 2005, 72, .	1.1	64
41	A Machine Learning Approach for the Prediction of Formability and Thermodynamic Stability of Single and Double Perovskite Oxides. Chemistry of Materials, 2021, 33, 845-858.	3.2	64
42	Nonlinear stability of $E$ centers in $Si$ Electronic structure calculations. Physical Review B, 2008, 78, .	1.1	63
43	Band-Gap and Band-Edge Engineering of Multicomponent Garnet Scintillators from First Principles. Physical Review Applied, 2015, 4, .	1.5	62
44	Opposite correlations between cation disordering and amorphization resistance in spinels versus pyrochlores. Nature Communications, 2015, 6, 8750.	5.8	62
45	Determining the site preference of trivalent dopants in bixbyite sesquioxides by atomic-scale simulations. Physical Review B, 2007, 75, .	1.1	61
46	Unprecedented irradiation resistance of nanocrystalline tungsten with equiaxed nanocrystalline grains to dislocation loop accumulation. Acta Materialia, 2019, 165, 118-128.	3.8	61
47	Tunable helium bubble superlattice ordered by screw dislocation network. Physical Review B, 2011, 84, .	1.1	58
48	Mechanistic materials modeling for nuclear fuel performance. Annals of Nuclear Energy, 2017, 105, 11-24.	0.9	57
49	Dynamical simulations of radiation damage in magnesium aluminate spinel, MgAl <sub>2</sub> O <sub>4</sub> . Journal of Physics Condensed Matter, 2005, 17, 875-891.	0.7	55
50	Predicted structure and stability of $A_4B_4$ phase compositions. Physical Review B, 2009, 80, .	1.1	54
51	Defect processes in MgAl <sub>2</sub> O <sub>4</sub> spinel. Solid State Sciences, 2008, 10, 717-724.	1.5	53
52	Thermodynamics of fission products in UO <sub>2</sub> . Journal of Physics Condensed Matter, 2009, 21, 435602.	0.7	52
53	Simulation of growth of Cu on Ag(001) at experimental deposition rates. Physical Review B, 2002, 66, .	1.1	51
54	Phosphorous clustering in germanium-rich silicon germanium. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2008, 154-155, 72-75.	1.7	51

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55	The mobility of small vacancy/helium complexes in tungsten and its impact on retention in fusion-relevant conditions. <i>Scientific Reports</i> , 2017, 7, 2522.	1.6	50
56	Role of di-interstitial clusters in oxygen transport in $\text{UO}_2$ first principles. <i>Physical Review B</i> , 2009, 80, .	1.1	49
57	Segregation of xenon to dislocations and grain boundaries in uranium dioxide. <i>Physical Review B</i> , 2011, 84, .	1.1	49
58	Multifidelity Information Fusion with Machine Learning: A Case Study of Dopant Formation Energies in Hafnia. <i>ACS Applied Materials &amp; Interfaces</i> , 2019, 11, 24906-24918.	4.0	49
59	First-principles DFT modeling of nuclear fuel materials. <i>Journal of Materials Science</i> , 2012, 47, 7367-7384.	1.7	47
60	Predicting lattice parameter as a function of cation disorder in MgAl <sub>2</sub> O <sub>4</sub> spinel. <i>Journal of Physics Condensed Matter</i> , 2005, 17, 7621-7631.	0.7	46
61	Microstructure, chemistry and mechanical properties of Ni-based superalloy Rene N4 under irradiation at room temperature. <i>Acta Materialia</i> , 2015, 95, 357-365.	3.8	46
62	Prediction of structure and cation ordering in an ordered normal-inverse double spinel. <i>Communications Materials</i> , 2020, 1, .	2.9	46
63	The Modern Temperature-Accelerated Dynamics Approach. <i>Annual Review of Chemical and Biomolecular Engineering</i> , 2016, 7, 87-110.	3.3	45
64	Models and simulations of nuclear fuel materials properties. <i>Journal of Alloys and Compounds</i> , 2007, 444-445, 415-423.	2.8	42
65	Machine learning in nuclear materials research. <i>Current Opinion in Solid State and Materials Science</i> , 2022, 26, 100975.	5.6	42
66	Defects in rutile and anatase polymorphs of TiO <sub>2</sub> : kinetics and thermodynamics near grain boundaries. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 435004.	0.7	40
67	Mechanism for transient migration of xenon in UO <sub>2</sub> . <i>Applied Physics Letters</i> , 2011, 98, .	1.5	40
68	Mobility and coalescence of stacking fault tetrahedra in Cu. <i>Scientific Reports</i> , 2015, 5, 9084.	1.6	40
69	Cation diffusion in magnesium aluminate spinel. <i>Solid State Ionics</i> , 2009, 180, 1-8.	1.3	39
70	Termination chemistry-driven dislocation structure at SrTiO <sub>3</sub> /MgO heterointerfaces. <i>Nature Communications</i> , 2014, 5, 5043.	5.8	39
71	Reduced grain boundary energies in rare-earth doped MgAl <sub>2</sub> O <sub>4</sub> spinel and consequent grain growth inhibition. <i>Journal of the European Ceramic Society</i> , 2017, 37, 4043-4050.	2.8	38
72	In-situ irradiation tolerance investigation of high strength ultrafine tungsten-titanium carbide alloy. <i>Acta Materialia</i> , 2019, 164, 547-559.	3.8	37

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73	Mechanism for recombination of radiation-induced point defects at interphase boundaries. <i>Physical Review B</i> , 2012, 85, .	1.1	36
74	Coupled motion of grain boundaries in bcc tungsten as a possible radiation-damage healing mechanism under fusion reactor conditions. <i>Nuclear Fusion</i> , 2013, 53, 063001.	1.6	36
75	Interface Energies of Nanocrystalline Doped Ceria: Effects of Manganese Segregation. <i>Journal of Physical Chemistry C</i> , 2015, 119, 27855-27864.	1.5	36
76	High-throughput investigation of the formation of double spinels. <i>Journal of Materials Chemistry A</i> , 2020, 8, 25756-25767.	5.2	36
77	Interface-enhanced defect absorption between epitaxial anatase TiO <sub>2</sub> film and single crystal SrTiO <sub>3</sub> . <i>Scripta Materialia</i> , 2011, 65, 807-810.	2.6	35
78	Formation of helium-bubble networks in tungsten. <i>Acta Materialia</i> , 2018, 159, 46-50.	3.8	35
79	Atomistic simulations of radiation-induced defect formation in spinels: MgAl <sub>2</sub> O <sub>4</sub> , MgGa <sub>2</sub> O <sub>4</sub> , and MgIn <sub>2</sub> O <sub>4</sub> . <i>Physical Review B</i> , 2006, 74, .	1.1	34
80	Simulation of defects and defect processes in fluorite and fluorite related oxides: Implications for radiation tolerance. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2007, 255, 151-157.	0.6	34
81	Parallel replica dynamics for driven systems: Derivation and application to strained nanotubes. <i>Physical Review B</i> , 2007, 75, .	1.1	34
82	Temperature accelerated dynamics study of migration process of oxygen defects in UO <sub>2</sub> . <i>Journal of Nuclear Materials</i> , 2009, 384, 315-321.	1.3	34
83	Stability and migration of large oxygen clusters in UO <sub>2</sub> : Density functional theory calculations. <i>Journal of Chemical Physics</i> , 2012, 136, 234702.	1.2	34
84	Multi-timescale investigation of radiation damage near TiO <sub>2</sub> /rutile grain boundaries. <i>Philosophical Magazine</i> , 2012, 92, 1469-1498.	0.7	34
85	Structural vs. intrinsic carriers: contrasting effects of cation chemistry and disorder on ionic conductivity in pyrochlores. <i>Journal of Materials Chemistry A</i> , 2015, 3, 11554-11565.	5.2	34
86	Massive Interfacial Reconstruction at Misfit Dislocations in Metal/Oxide Interfaces. <i>Scientific Reports</i> , 2014, 4, 6533.	1.6	34
87	Temperature dependence of the radiation tolerance of nanocrystalline pyrochlores A <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub> (A = Gd, Ho). <i>Journal of Nuclear Energy Part B</i> , 2014, 100, 1-10.	1.1	34
88	Interstitial and vacancy mediated transport mechanisms in perovskites: A comparison of chemistry and potentials. <i>Solid State Ionics</i> , 2013, 253, 18-26.	1.3	33
89	Structure and segregation of dopant-defect complexes at grain boundaries in nanocrystalline doped ceria. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15375-15385.	1.3	33
90	Stabilization of MgAl <sub>2</sub> O <sub>4</sub> spinel surfaces via doping. <i>Surface Science</i> , 2016, 649, 138-145.	0.8	33

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91	Using Machine Learning To Identify Factors That Govern Amorphization of Irradiated Pyrochlores. Chemistry of Materials, 2017, 29, 2574-2583.	3.2	33
92	Mechanisms and Rates of Interstitial H <sub>2</sub> Diffusion in Crystalline C <sub>60</sub> . Physical Review Letters, 2003, 91, 105901.	2.9	32
93	Effect of Cation Ordering on Oxygen Vacancy Diffusion Pathways in Double Perovskites. Chemistry of Materials, 2015, 27, 5020-5026.	3.2	32
94	Multiscale simulation of xenon diffusion and grain boundary segregation in UO <sub>2</sub> . Journal of Nuclear Materials, 2015, 462, 15-25.	1.3	32
95	Simulation of radiation driven fission gas diffusion in UO <sub>2</sub> , ThO <sub>2</sub> and PuO <sub>2</sub> . Journal of Nuclear Materials, 2016, 481, 125-133.	1.3	32
96	A new mechanism for void-cascade interaction from nondestructive depth-resolved atomic-scale measurements of ion irradiation-induced defects in Fe. Science Advances, 2020, 6, eaba8437.	4.7	32
97	Molecular dynamics modelling of radiation damage in normal, partly inverse and inverse spinels. Nuclear Instruments & Methods in Physics Research B, 2006, 250, 36-45.	0.6	30
98	Diffusion of small self-interstitial clusters in silicon: Temperature-accelerated tight-binding molecular dynamics simulations. Physical Review B, 2005, 71, .	1.1	29
99	Reaching extended length scales and time scales in atomistic simulations via spatially parallel temperature-accelerated dynamics. Physical Review B, 2007, 76, .	1.1	29
100	Engineering the free vacancy and active donor concentrations in phosphorus and arsenic double donor-doped germanium. Journal of Applied Physics, 2008, 104, .	1.1	29
101	The effect of Ga-doping on the defect chemistry of RE <sub>3</sub> Al <sub>5</sub> O <sub>12</sub> garnets. Physica Status Solidi (B): Basic Research, 2013, 250, 244-248.	0.7	29
102	Method to account for arbitrary strains in kinetic Monte Carlo simulations. Physical Review B, 2013, 87, .	1.1	29
103	The interaction of a screw dislocation with point defects in bcc iron. Philosophical Magazine, 2012, 92, 2759-2778.	0.7	28
104	Interaction of small mobile stacking fault tetrahedra with free surfaces, dislocations, and interfaces in Cu and Cu-Nb. Physical Review B, 2016, 93, .	1.1	28
105	Evidence for percolation diffusion of cations and reordering in disordered pyrochlore from accelerated molecular dynamics. Nature Communications, 2017, 8, 618.	5.8	28
106	Physics-informed machine learning for inorganic scintillator discovery. Journal of Chemical Physics, 2018, 148, 241729.	1.2	28
107	Defect identification and compensation in rare earth oxide scintillators. Nuclear Instruments & Methods in Physics Research B, 2008, 266, 2657-2664.	0.6	27
108	Impact of homogeneous strain on uranium vacancy diffusion in uranium dioxide. Physical Review B, 2015, 91, .	1.1	27

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109	Improving the Thermodynamic Stability of Aluminate Spinel Nanoparticles with Rare Earths. Chemistry of Materials, 2016, 28, 5163-5171.	3.2	27
110	Onset conditions for flash sintering of UO <sub>2</sub> . Journal of Nuclear Materials, 2017, 493, 264-270.	1.3	27
111	Atomistic modeling of out-of-pile xenon diffusion by vacancy clusters in UO <sub>2</sub> . Journal of Nuclear Materials, 2019, 520, 96-109.	1.3	27
112	Effects of Radiation-Induced Defects on Corrosion. Annual Review of Materials Research, 2021, 51, 293-328.	4.3	27
113	Point defect thermodynamics and diffusion in Fe <sub>3</sub> C: A first-principles study. Acta Materialia, 2008, 56, 3236-3244.	3.8	26
114	Parallel replica dynamics with a heterogeneous distribution of barriers: Application to hexadecane pyrolysis. Journal of Chemical Physics, 2004, 121, 9808-9819.	1.2	25
115	Predicting from first principles the chemical evolution of crystalline compounds due to radioactive decay: The case of the transformation of CsCl to BaCl. Physical Review B, 2009, 79, .	1.1	25
116	Grain boundary stoichiometry and interactions with defects in SrTiO <sub>3</sub> . Scripta Materialia, 2012, 66, 105-108.	2.6	25
117	Linking Interfacial Step Structure and Chemistry with Locally Enhanced Radiation-Induced Amorphization at Oxide Heterointerfaces. Advanced Materials Interfaces, 2014, 1, 1300142.	1.9	25
118	Atomistic study of the dissolution of small boron interstitial clusters in c-Si. Applied Physics Letters, 2005, 87, 191912.	1.5	24
119	Vacancy Formation and Strain in Low-Temperature $\text{Cu} < \text{mml:mn} > 100 < \text{mml:mn} > \text{Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 327 Td (stretchy="false"}$	2.9	24
120	Radiation damage at the coherent anatase interface under Ne ion irradiation. Journal of Nuclear Materials, 2012, 429, 177-184.	1.3	24
121	Point defect-grain boundary interactions in MgO: an atomistic study. Journal of Physics Condensed Matter, 2013, 25, 355001.	0.7	24
122	Stress-induced phase transformation in nanocrystalline UO <sub>2</sub> . Scripta Materialia, 2009, 60, 878-881.	2.6	23
123	Order-to-disorder phase transformation in ion irradiated uranium-bearing delta-phase oxides RE <sub>6</sub> U <sub>10</sub> O <sub>12</sub> (RE=Y, Gd, Ho, Yb, and Lu). Journal of Solid State Chemistry, 2010, 183, 844-848.	1.4	23
124	Role of Sink Density in Nonequilibrium Chemical Redistribution in Alloys. Physical Review Letters, 2018, 120, 106101.	2.9	23
125	Massively enhanced ionic transport in irradiated crystalline pyrochlore. Journal of Materials Chemistry A, 2019, 7, 3917-3923.	5.2	23
126	Distortion-stabilized ordered structures in A <sub>2</sub> B <sub>2</sub> O <sub>7</sub> mixed pyrochlores. Npj Computational Materials, 2019, 5, .	3.5	23



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127	Accelerated dynamics study of vacancy mobility in $\alpha$ -plutonium. <i>Journal of Alloys and Compounds</i> , 2007, 444-445, 314-319.	2.8	22
128	Intrinsic electrostatic effects in nanostructured ceramics. <i>Physical Review B</i> , 2010, 81, .	1.1	22
129	Resilient ZnO nanowires in an irradiation environment: An in situ study. <i>Acta Materialia</i> , 2015, 95, 156-163.	3.8	22
130	Anion order in oxysulfide perovskites: origins and implications. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	22
131	Theoretical Studies of Self-Diffusion and Dopant Clustering in Semiconductors. <i>Physica Status Solidi (B): Basic Research</i> , 2002, 233, 24-30.	0.7	21
132	Radiation damage in heteroepitaxial BaTiO <sub>3</sub> thin films on SrTiO <sub>3</sub> under Ne ion irradiation. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	21
133	Defect interactions with stepped CeO <sub>2</sub> /SrTiO <sub>3</sub> interfaces: Implications for radiation damage evolution and fast ion conduction. <i>Journal of Chemical Physics</i> , 2014, 140, 194701.	1.2	21
134	Non-uniform Solute Segregation at Semi-Coherent Metal/Oxide Interfaces. <i>Scientific Reports</i> , 2015, 5, 13086.	1.6	21
135	The thermodynamic and kinetic interactions of He interstitial clusters with bubbles in W. <i>Journal of Applied Physics</i> , 2016, 119, .	1.1	21
136	The role of surfaces, chemical interfaces, and disorder on plutonium incorporation in pyrochlores. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22852-22863.	1.3	21
137	Elastic sheet method for identifying atoms in molecules. <i>Journal of Chemical Physics</i> , 1999, 111, 10664-10669.	1.2	20
138	Exploring long-time response to radiation damage in MgO. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2005, 228, 260-273.	0.6	20
139	Using $\alpha$ -radioparagenesis to design robust nuclear waste forms. <i>Energy and Environmental Science</i> , 2010, 3, 130-135.	15.6	20
140	Cation disorder in MgX <sub>2</sub> O <sub>4</sub> (X= Al, Ga, In) spinels from first principles. <i>Physical Review B</i> , 2012, 86, .	1.1	20
141	The role of charge and ionic radius on fission product segregation to a model UO <sub>2</sub> grain boundary. <i>Journal of Applied Physics</i> , 2013, 113, .	1.1	20
142	Irradiation-induced grain growth and defect evolution in nanocrystalline zirconia with doped grain boundaries. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16921-16929.	1.3	20
143	New helium bubble growth mode at a symmetric grain-boundary in tungsten: accelerated molecular dynamics study. <i>Materials Research Letters</i> , 2018, 6, 522-530.	4.1	20
144	Growth Rate Effects on the Formation of Dislocation Loops Around Deep Helium Bubbles in Tungsten. <i>Fusion Science and Technology</i> , 2017, 71, 1-6.	0.6	20

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145	Defect structure of ZrO <sub>2</sub> -doped rare earth perovskite scintillators. <i>Physica Status Solidi (B): Basic Research</i> , 2005, 242, R113-R115.	0.7	19
146	Radiation damage and evolution of radiation-induced defects in Er <sub>2</sub> O <sub>3</sub> bixbyite. <i>Journal of Physics Condensed Matter</i> , 2009, 21, 115403.	0.7	19
147	Defect Distributions and Transport in Nanocomposites: A Theoretical Perspective. <i>Materials Research Letters</i> , 2013, 1, 193-199.	4.1	19
148	Atomic-Scale Structure and Stability of the Low-Index Surfaces of Pyrochlore Oxides. <i>Journal of Physical Chemistry C</i> , 2016, 120, 10485-10499.	1.5	19
149	Semicoherent oxide heterointerfaces: Structure, properties, and implications. <i>APL Materials</i> , 2019, 7, .	2.2	19
150	Band-Edge Engineering To Eliminate Radiation-Induced Defect States in Perovskite Scintillators. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 46296-46305.	4.0	19
151	Defect behavior in oxides: Insights from modern atomistic simulation methods. <i>Current Opinion in Solid State and Materials Science</i> , 2013, 17, 249-256.	5.6	18
152	Insights into dynamic processes of cations in pyrochlores and other complex oxides. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 24215-24223.	1.3	18
153	Thermodynamics of fission products in dispersion fuel designs – First-principles modeling of defect behavior in bulk and at interfaces. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2010, 268, 3014-3017.	0.6	17
154	Radioparagenesis: The formation of novel compounds and crystalline structures via radioactive decay. <i>Philosophical Magazine Letters</i> , 2010, 90, 435-446.	0.5	17
155	Chemical evolution via beta decay: a case study in strontium-90. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 065504.	0.7	17
156	Irradiation effects in an HfO <sub>2</sub> /MgO/HfO <sub>2</sub> tri-layer structure induced by 10 MeV Au ions. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2009, 267, 1918-1923.	0.6	16
157	First-principles localized cluster expansion study of the kinetics of hydrogen diffusion in homogeneous and heterogeneous Fe-Cr alloys. <i>Physical Review B</i> , 2019, 99, .	1.1	16
158	Solubility and clustering of ruthenium fission products in uranium dioxide as determined by density functional theory. <i>Physical Review B</i> , 2012, 85, .	1.1	15
159	Interpreting oxygen vacancy migration mechanisms in oxides using the layered structure motif. <i>Computational Materials Science</i> , 2015, 103, 216-223.	1.4	15
160	Role of Multiple Charge States of $Ce$ in the Scintillation of $AB_3O_3$	1.5	15
161	Implications of transmutation on the defect chemistry in crystalline waste forms. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2010, 268, 3261-3264.	0.6	14
162	Influence of point defects on grain boundary mobility in bcc tungsten. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 035402.	0.7	14

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163	Orientation-specific amorphization and intercalated recrystallization at ion-irradiated SrTiO <sub>3</sub> /MgO interfaces. Journal of Materials Research, 2014, 29, 1699-1710.	1.2	14
164	Ideal sinks are not always ideal: Radiation damage accumulation in nanocomposites. Journal of Nuclear Materials, 2015, 462, 402-408.	1.3	14
165	Swift heavy ion irradiation-induced microstructure modification of two delta-phase oxides: Sc <sub>4</sub> Zr <sub>3</sub> O <sub>12</sub> and Lu <sub>4</sub> Zr <sub>3</sub> O <sub>12</sub> . Nuclear Instruments & Methods in Physics Research B, 2010, 268, 3243-3247.	0.6	13
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