

# Michael Finnis

## List of Publications by Citations

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169  
papers

11,012  
citations

52  
h-index

103  
g-index

175  
ext. papers

11,787  
ext. citations

5.3  
avg, IF

6.19  
L-index

#	Paper	IF	Citations
169	A simple empirical N-body potential for transition metals. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>1984</b> , 50, 45-55		2630
168	Simple N-body potentials for the noble metals and nickel. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>1987</b> , 56, 735-756		524
167	The theory of metal - ceramic interfaces. <i>Journal of Physics Condensed Matter</i> , <b>1996</b> , 8, 5811-5836	1.8	426
166	The tight-binding bond model. <i>Journal of Physics C: Solid State Physics</i> , <b>1988</b> , 21, 35-66		383
165	Long range interactions in nanoscale science. <i>Reviews of Modern Physics</i> , <b>2010</b> , 82, 1887-1944	40.5	304
164	Theory of lattice contraction at aluminium surfaces. <i>Journal of Physics F: Metal Physics</i> , <b>1974</b> , 4, L37-L41		296
163	A stabilization mechanism of zirconia based on oxygen vacancies only. <i>Acta Materialia</i> , <b>2002</b> , 50, 5171-5188		262
162	Thermal excitation of electrons in energetic displacement cascades. <i>Physical Review B</i> , <b>1991</b> , 44, 567-574	3.3	171
161	Semi-empirical calculation of solid surface tensions in body-centred cubic transition metals. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>1986</b> , 54, 301-315		169
160	The influence of grain boundary inclination on the structure and energy of $\Sigma$ 3 grain boundaries in copper. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>1992</b> , 66, 991-1016		167
159	Magnetism and thermodynamics of defect-free Fe-Cr alloys. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	162
158	Supercell size scaling of density functional theory formation energies of charged defects. <i>Physical Review B</i> , <b>2009</b> , 79,	3.3	154
157	First-Principles Calculations of the Ideal Cleavage Energy of Bulk Niobium(111)/Alumina(0001) Interfaces. <i>Physical Review Letters</i> , <b>1999</b> , 82, 1510-1513	7.4	154
156	Equilibrium and adhesion of Nb/sapphire: The effect of oxygen partial pressure. <i>Physical Review B</i> , <b>2000</b> , 62, 4698-4706	3.3	147
155	SrTiO <sub>3</sub> (001)(2 $\times$ 1) reconstructions: First-principles calculations of surface energy and atomic structure compared with scanning tunneling microscopy images. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	145
154	Bismuth embrittlement of copper is an atomic size effect. <i>Nature</i> , <b>2004</b> , 432, 1008-11	50.4	145
153	Theoretical prediction and direct observation of the 9R structure in Ag. <i>Physical Review Letters</i> , <b>1992</b> , 69, 620-623	7.4	135

152	THE OXIDATION OF NIAL: What Can We Learn from Ab Initio Calculations?. <i>Annual Review of Materials Research</i> , <b>2005</b> , 35, 167-207	12.8	112
151	Ab initio calculations on the Al <sub>2</sub> O <sub>3</sub> (0001) surface. <i>Faraday Discussions</i> , <b>1999</b> , 114, 33-43	3.6	112
150	Structural and chemical embrittlement of grain boundaries by impurities: A general theory and first-principles calculations for copper. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	108
149	Crystal Structures of Zirconia from First Principles and Self-Consistent Tight Binding. <i>Physical Review Letters</i> , <b>1998</b> , 81, 5149-5152	7.4	108
148	Irradiation creep models An overview. <i>Journal of Nuclear Materials</i> , <b>1988</b> , 159, 257-285	3.3	107
147	The energy and elastic constants of simple metals in terms of pairwise interactions. <i>Journal of Physics F: Metal Physics</i> , <b>1974</b> , 4, 1645-1656		106
146	On the growth of Al <sub>2</sub> O <sub>3</sub> scales. <i>Acta Materialia</i> , <b>2013</b> , 61, 6670-6683	8.4	103
145	Validity of the second moment tight-binding model. <i>Journal of Physics F: Metal Physics</i> , <b>1988</b> , 18, L153-L157		103
144	Metal-ceramic cohesion and the image interaction. <i>Acta Metallurgica Et Materialia</i> , <b>1992</b> , 40, S25-S37		102
143	Prediction of high-temperature point defect formation in TiO <sub>2</sub> from combined ab initio and thermodynamic calculations. <i>Acta Materialia</i> , <b>2007</b> , 55, 4325-4337	8.4	101
142	The treatment of electronic excitations in atomistic models of radiation damage in metals. <i>Reports on Progress in Physics</i> , <b>2010</b> , 73, 116501	14.4	91
141	Surface structure and water adsorption on Fe <sub>3</sub> O <sub>4</sub> (111): Spin-density functional theory and on-site Coulomb interactions. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	88
140	Atom probe tomography analysis of the distribution of rhenium in nickel alloys. <i>Acta Materialia</i> , <b>2010</b> , 58, 931-942	8.4	84
139	Point defects and chemical potentials in ordered alloys. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>1998</b> , 77, 447-464		83
138	The Harris functional applied to surface and vacancy formation energies in aluminium. <i>Journal of Physics Condensed Matter</i> , <b>1990</b> , 2, 331-342	1.8	77
137	Relative energetics and structural properties of zirconia using a self-consistent tight-binding model. <i>Physical Review B</i> , <b>2000</b> , 61, 6617-6630	3.3	76
136	Solid-liquid interface free energy through metadynamics simulations. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	69
135	The interaction of a point charge with an aluminium (111) surface. <i>Surface Science</i> , <b>1991</b> , 241, 61-72	1.8	69

134	On the possibility of rhenium clustering in nickel-based superalloys. <i>Acta Materialia</i> , <b>2012</b> , 60, 2866-2878.	8.4	67
133	Atomistic study of structural correlations at a liquid-solid interface. <i>Computational Materials Science</i> , <b>2002</b> , 24, 443-452	3.2	65
132	Surface stoichiometry and the initial oxidation of NiAl(110). <i>Physical Review Letters</i> , <b>2000</b> , 85, 610-3	7.4	65
131	Vacancy formation energies and linear screening theory. <i>Journal of Physics F: Metal Physics</i> , <b>1976</b> , 6, 483-498		63
130	Ab initio atomistic simulation of the strength of defective aluminum and tests of empirical force models. <i>Physical Review B</i> , <b>1995</b> , 52, 15191-15207	3.3	61
129	Improved method of calculating ab initio high-temperature thermodynamic properties with application to ZrC. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	60
128	Interatomic potentials for strontium titanate: An assessment of their transferability and comparison with density functional theory. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	60
127	Interatomic forces in transition metals. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>1988</b> , 58, 143-163		59
126	Free energy and molecular dynamics calculations for the cubic-tetragonal phase transition in zirconia. <i>Physical Review B</i> , <b>2001</b> , 63,	3.3	57
125	First-Principles Calculations for Niobium Atoms on a Sapphire Surface. <i>Journal of the American Ceramic Society</i> , <b>1994</b> , 77, 431-436	3.8	57
124	Vacancy formation volumes in simple metals. <i>Journal of Physics F: Metal Physics</i> , <b>1976</b> , 6, 965-978		57
123	Prediction and observation of the bcc structure in pure copper at a Sigma 3 grain boundary. <i>Physical Review Letters</i> , <b>1995</b> , 75, 2160-2163	7.4	55
122	Accessing the Excess: An Atomistic Approach to Excesses at Planar Defects and Dislocations in Ordered Compounds. <i>Physica Status Solidi A</i> , <b>1998</b> , 166, 397-416		54
121	Transferable atomistic model to describe the energetics of zirconia. <i>Physical Review B</i> , <b>1996</b> , 54, 9147-9161	3.3	54
120	Interatomic Forces and Phonon Anomalies in bcc 3d Transition Metals. <i>Physical Review Letters</i> , <b>1984</b> , 52, 291-294	7.4	54
119	A critique of rhenium clustering in NiBe alloys using extended X-ray absorption spectroscopy. <i>Acta Materialia</i> , <b>2008</b> , 56, 2669-2675	8.4	52
118	A calculation of elastic constants of ferromagnetic iron at finite temperatures. <i>Journal of Physics F: Metal Physics</i> , <b>1985</b> , 15, 19-34		52
117	Electron energy-loss near-edge shape as a probe to investigate the stabilization of yttria-stabilized zirconia. <i>Physical Review B</i> , <b>2002</b> , 65,	3.3	51

116	Theoretical and experimental investigations of structures and energies of $\Sigma$ 3, [112] tilt grain boundaries in copper. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>1998</b> , 77, 1161-1184		49
115	First-principles study of the atomistic and electronic structure of the niobium--alumina (0001) interface. <i>Philosophical Magazine Letters</i> , <b>1996</b> , 73, 377-384	1	49
114	Plasmonic ELISA for the detection of gp120 at ultralow concentrations with the naked eye. <i>Nanoscale</i> , <b>2014</b> , 6, 9559-62	7.7	48
113	Analytic bond-order potentials for multicomponent systems. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , <b>2004</b> , 365, 2-13	5.3	48
112	Ordering at Solid-Liquid Interfaces Between Dissimilar Materials. <i>Journal of Materials Science</i> , <b>2001</b> , 9, 175-181		46
111	Effect of relaxation on the oxygen K-edge electron energy-loss near-edge structure in yttria-stabilized zirconia. <i>Physical Review B</i> , <b>2000</b> , 62, 14728-14735	3.3	46
110	First-Principles Approach to Model Electrochemical Reactions: Understanding the Fundamental Mechanisms behind Mg Corrosion. <i>Physical Review Letters</i> , <b>2018</b> , 120, 246801	7.4	45
109	Perspectives on point defect thermodynamics. <i>Physica Status Solidi (B): Basic Research</i> , <b>2014</b> , 251, 97-129.	1.3	45
108	Insight into gallium behavior in aluminum grain boundaries from calculation on $\Sigma$ 11 (113) boundary. <i>Acta Materialia</i> , <b>2000</b> , 48, 3623-3632	8.4	44
107	Transferable model for the atomistic simulation of Al <sub>2</sub> O <sub>3</sub> . <i>Physical Review B</i> , <b>1996</b> , 54, 15683-15689	3.3	44
106	Sputtering of gold foils in a high voltage electron microscope A comparison of theory and experiment. <i>Philosophical Magazine and Journal</i> , <b>1977</b> , 35, 693-714		44
105	Interstitials in FeCr alloys studied by density functional theory. <i>Physical Review B</i> , <b>2007</b> , 76,	3.3	43
104	Theoretical and experimental analysis of near $\Sigma$ (211) boundaries in silver. <i>Acta Metallurgica Et Materialia</i> , <b>1994</b> , 42, 3555-3567		43
103	Atomistic and electronic structure of Al/MgAl <sub>2</sub> O <sub>4</sub> and Ag/MgAl <sub>2</sub> O <sub>4</sub> interfaces. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>2001</b> , 81, 927-955		42
102	The Structure of Grain Boundaries in Strontium Titanate: Theory, Simulation, and Electron Microscopy. <i>Annual Review of Materials Research</i> , <b>2010</b> , 40, 557-599	12.8	40
101	The Band Structure of Polycrystalline Al <sub>2</sub> O <sub>3</sub> and Its Influence on Transport Phenomena. <i>Journal of the American Ceramic Society</i> , <b>2016</b> , 99, 733-747	3.8	35
100	Magnetic tight binding and the iron-chromium enthalpy anomaly. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	34
99	Ab initio calculations of metal/ceramic interfaces: what have we learned, what can we learn?. <i>Scripta Materialia</i> , <b>1995</b> , 6, 145-155		33

98	Anomalous diffusion along metal/ceramic interfaces. <i>Nature Communications</i> , <b>2018</b> , 9, 5251	17.4	33
97	Electronic damping of atomic dynamics in irradiation damage of metals. <i>Journal of Physics Condensed Matter</i> , <b>2007</b> , 19, 436209	1.8	30
96	Why TiC(111) is observed to be Ti terminated. <i>Surface Science</i> , <b>1996</b> , 348, 49-54	1.8	30
95	The structure of special grain boundaries in $\beta$ -Al <sub>2</sub> O <sub>3</sub> . <i>Journal of Physics and Chemistry of Solids</i> , <b>1994</b> , 55, 1067-1082	3.9	30
94	Energetics of charged point defects in rutile TiO <sub>2</sub> by density functional theory. <i>Acta Materialia</i> , <b>2009</b> , 57, 5882-5891	8.4	29
93	Determination of the Atomistic Structure of the $\beta$ (111) Twin Boundary in NiAl. <i>Materials Science Forum</i> , <b>1996</b> , 207-209, 245-248	0.4	29
92	Bond-order potentials through the ages. <i>Progress in Materials Science</i> , <b>2007</b> , 52, 133-153	42.2	28
91	The interaction of a point charge with a metal surface: theory and calculations for (111), (100) and (110) aluminium surfaces. <i>Journal of Physics Condensed Matter</i> , <b>1995</b> , 7, 2001-2019	1.8	28
90	The energy of helium filled platelets and bubbles in molybdenum. <i>Radiation Effects</i> , <b>1983</b> , 78, 121-132		28
89	Pressure-Induced Isostructural Phase Transition in Al-Rich NiAl Alloys. <i>Physical Review Letters</i> , <b>1999</b> , 83, 979-982	7.4	27
88	Energetic and kinetic aspects of the faceting transformation of a $\beta$ grain boundary in Cu. <i>Acta Metallurgica Et Materialia</i> , <b>1993</b> , 41, 2163-2171		27
87	A comparison of methods for calculating tight-binding bond energies. <i>Journal of Physics F: Metal Physics</i> , <b>1988</b> , 18, 693-718		26
86	Electronic structures and phonon free energies of LaCoO <sub>3</sub> using hybrid-exchange density functional theory. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	25
85	Surface energy and the early stages of oxidation of NiAl(110). <i>Computer Physics Communications</i> , <b>2001</b> , 137, 174-194	4.2	25
84	Oxygen vacancy formation energies in Sr-doped complex perovskites: ab initio thermodynamic study. <i>Solid State Ionics</i> , <b>2014</b> , 254, 11-16	3.3	24
83	Stability of Sr adatom model structures for SrTiO <sub>3</sub> (001) surface reconstructions. <i>Journal of Physics Condensed Matter</i> , <b>2005</b> , 17, L223-L230	1.8	24
82	Bond energies and defect forces around a vacancy in BCC transition metals. <i>Journal of Physics F: Metal Physics</i> , <b>1987</b> , 17, L273-L281		24
81	The diffusion of doxorubicin drug molecules in silica nanoslits is non-Gaussian, intermittent and anticorrelated. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 27955-27965	3.6	24

80	A simple theory of some phase transitions. <i>Journal of Physics F: Metal Physics</i> , <b>1974</b> , 4, 960-968		23
79	A Density Functional Study of Interactions at the Metal/Ceramic Interfaces Al/MgAl <sub>2</sub> O <sub>4</sub> and Ag/MgAl <sub>2</sub> O <sub>4</sub> . <i>Physica Status Solidi A</i> , <b>1998</b> , 166, 417-428		22
78	Atomistic study of ordinary screw dislocations in single-phase and lamellar $\beta$ -TiAl. <i>Philosophical Magazine</i> , <b>2007</b> , 87, 1795-1809	1.6	21
77	Heat of transport in solids. III. Computer simulation of vacancy in an FCC crystal. <i>Journal of Physics C: Solid State Physics</i> , <b>1978</b> , 11, 4469-4483		21
76	Plutonium redistribution in mixed oxide (U, Pu)O <sub>2</sub> nuclear fuel elements. <i>Journal of Nuclear Materials</i> , <b>1978</b> , 75, 193-200	3.3	20
75	Structure of multilayer ZrO <sub>2</sub> /SrTiO <sub>3</sub> . <i>Journal of Materials Science</i> , <b>2012</b> , 47, 1631-1640	4.3	19
74	Ab initio computational study of Ga in an Al grain boundary. <i>Philosophical Magazine Letters</i> , <b>1997</b> , 76, 281-288	1	19
73	Phonon softening in ferromagnetic BCC iron. <i>Journal of Physics F: Metal Physics</i> , <b>1987</b> , 17, 2049-2055		19
72	Defect energies and linear screening theory in simple metals. <i>Journal of Physics F: Metal Physics</i> , <b>1975</b> , 5, 2227-2240		19
71	MEAMfit: A reference-free modified embedded atom method (RF-MEAM) energy and force-fitting code. <i>Computer Physics Communications</i> , <b>2015</b> , 196, 439-445	4.2	18
70	The role of ceramic and glass science research in meeting societal challenges: Report from an NSF-sponsored workshop. <i>Journal of the American Ceramic Society</i> , <b>2017</b> , 100, 1777-1803	3.8	17
69	Atomic-scale characterization of the SrTiO <sub>3</sub> B(112)[1 $\bar{1}$ 0] grain boundary. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	16
68	The $\beta$ -alumina(0001) surface: relaxations and dynamics from shell model and density functional theory. <i>Journal of the European Ceramic Society</i> , <b>2003</b> , 23, 2729-2735	6	16
67	Ab initio transmission electron microscopy image simulations of coherent Ag/MgO interfaces. <i>Physical Review B</i> , <b>2004</b> , 70,	3.3	15
66	Interatomic forces in materials. <i>Progress in Materials Science</i> , <b>2004</b> , 49, 1-18	42.2	15
65	The temperature dependence of the Debye-Waller factors of B <sub>2</sub> NiAl. <i>Philosophical Magazine Letters</i> , <b>1996</b> , 73, 137-144	1	15
64	Structural and electronic properties of $\beta$ grain boundaries in $\beta$ -Al <sub>2</sub> O <sub>3</sub> . <i>Acta Materialia</i> , <b>2015</b> , 99, 16-28	8.4	14
63	A physically transparent and transferable compressible ion model for oxides. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 4406	3.9	13

62	The role of the interface in determining the orientation of solid rare gas bubbles in metals. <i>Acta Metallurgica</i> , <b>1987</b> , 35, 2543-2547		13
61	Theory of vacancy formation volume. <i>Journal of Physics F: Metal Physics</i> , <b>1977</b> , 7, 1999-2010		13
60	Energies of defects in ordered alloys: dislocation core energies in NiAl. <i>Acta Materialia</i> , <b>1998</b> , 46, 919-926.	4	12
59	Correlated electron-ion dynamics in metallic systems. <i>Computational Materials Science</i> , <b>2008</b> , 44, 16-20	3.2	12
58	Migration mechanisms of a faceted grain boundary. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	12
57	Observations and theory of thermally-induced helium bubble shrinkage in gold. <i>Journal of Nuclear Materials</i> , <b>1989</b> , 168, 19-23	3.3	11
56	A theory of irradiation and thermal creep by dislocation climb. <i>Journal of Nuclear Materials</i> , <b>1981</b> , 104, 1263-1267	3.3	11
55	Quantum mechanical simulations of electronic stopping in metals. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , <b>2011</b> , 269, 1640-1645	1.2	10
54	Concepts for simulating and understanding materials at the atomic scale. <i>MRS Bulletin</i> , <b>2012</b> , 37, 477-484.	3.2	10
53	Dynamics and free energy of $\alpha$ -alumina (0001) surfaces: I. Semi-empirical model. <i>Journal of Physics Condensed Matter</i> , <b>2002</b> , 14, 7797-7810	1.8	10
52	Point defects and chemical potentials in ordered alloys		10
51	Crack-Tip Blunting Versus Cleavage Extension <b>1983</b> , 1047-1051		10
50	Ab initio based method to study structural phase transitions in dynamically unstable crystals, with new insights on the $\beta$ to $\alpha$ transformation in titanium. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	9
49	Atomistic force field for alumina fit to density functional theory. <i>Journal of Chemical Physics</i> , <b>2013</b> , 139, 204704	3.9	9
48	Electrostatic and Entropic Interactions between Parallel Interfaces Separated by a Glassy Film. <i>Journal of the American Ceramic Society</i> , <b>2002</b> , 85, 2562-2568	3.8	9
47	An isothermal-isobaric Langevin thermostat for simulating nanoparticles under pressure: application to Au clusters. <i>ChemPhysChem</i> , <b>2005</b> , 6, 1848-52	3.2	9
46	The challenges of hydrogen and metals. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , <b>2017</b> , 375,	3	8
45	Ab Initio Study of Electronic and Geometric Structures of Metal/Ceramic Heterophase Boundaries. <i>Materials Research Society Symposia Proceedings</i> , <b>1997</b> , 492, 97		8



44	Atomistic Simulation of Grain Boundaries in Alumina. <i>Materials Science Forum</i> , <b>1996</b> , 207-209, 225-228	0.4	8
43	Fast anharmonic free energy method with an application to vacancies in ZrC. <i>Physical Review B</i> , <b>2019</b> , 100,	3.3	7
42	Al-oxynitride interfacial layer investigations for PrXOYon SiC and Si. <i>Journal of Physics: Conference Series</i> , <b>2008</b> , 94, 012004	0.3	7
41	The movement of lenticular pores in mixed oxide (U, Pu) O2 nuclear fuel elements. <i>Journal of Nuclear Materials</i> , <b>1978</b> , 75, 115-124	3.3	7
40	Solid-liquid phase equilibria from free-energy perturbation calculations. <i>Physical Review B</i> , <b>2008</b> , 78,	3.3	5
39	Comment on "Metal-ceramic adhesion and the Harris functional". <i>Physical Review Letters</i> , <b>1995</b> , 74, 30837.4	4	5
38	Understanding adhesion between metal and oxide. <i>Materials at High Temperatures</i> , <b>1994</b> , 12, 189-194	1.1	5
37	Self-Consistent Tight-Binding Approximation Including Polarizable Ions. <i>Materials Research Society Symposia Proceedings</i> , <b>1997</b> , 491, 265		4
36	First principles investigation of polarisation at interfaces in multilayered strontium titanate. <i>Journal of Physics: Conference Series</i> , <b>2008</b> , 94, 012005	0.3	4
35	Studies of grain orientations and grain boundaries in polycrystalline SrTiO3. <i>Journal of Physics: Conference Series</i> , <b>2008</b> , 94, 012008	0.3	4
34	Changes in macroscopic behaviour through segregation in niobium doped strontium titanate. <i>Journal of Physics: Conference Series</i> , <b>2008</b> , 94, 012015	0.3	4
33	Representations of the local atomic density. <i>Journal of Physics Condensed Matter</i> , <b>1998</b> , 10, 7983-7993	1.8	4
32	The theory of distorted structures in the Cd-Mg and In-Tl alloy systems. <i>Journal of Physics F: Metal Physics</i> , <b>1974</b> , 4, 969-980		4
31	Grand canonical approach to modeling hydrogen trapping at vacancies in Be. <i>Physical Review Materials</i> , <b>2020</b> , 4,	3.2	4
30	Vacancy formation energies and volumes in simple metals. <i>Journal of Nuclear Materials</i> , <b>1978</b> , 69-70, 638-640	3.3	3
29	Spontaneous Frenkel pair formation in zirconium carbide. <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	3
28	Point Defects in NiAl Alloys Under Pressure <b>2000</b> , 439-454		3
27	Calculating Grain Boundary Energies and Other Defect Energies in Ordered Alloys <b>1997</b> , 339-347		3

26	Structure and ionic diffusivity in an yttria-stabilised zirconia/strontium titanate multilayer. <i>Acta Materialia</i> , <b>2017</b> , 129, 388-397	8.4	2
25	A model for time-dependent grain boundary diffusion of ions and electrons through a film or scale, with an application to alumina. <i>Acta Materialia</i> , <b>2017</b> , 132, 503-516	8.4	2
24	New methods for calculating the free energy of charged defects in solid electrolytes. <i>Journal of Physics Condensed Matter</i> , <b>2013</b> , 25, 395001	1.8	2
23	Aiding the Design of Radiation Resistant Materials with Multiphysics Simulations of Damage Processes. <i>Materials Research Society Symposia Proceedings</i> , <b>2009</b> , 1229, 30601		2
22	Bi <sub>3</sub> .25La <sub>0.75</sub> Ti <sub>3</sub> O <sub>12</sub> films on La <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub> thin films prepared by chemical solution deposition. <i>Journal of Physics: Conference Series</i> , <b>2008</b> , 94, 012014	0.3	2
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20	Improved representation of metallic bonding in atomistic simulations. <i>Philosophical Magazine Letters</i> , <b>1996</b> , 73, 39-44	1	2
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