Michael Finnis

List of Publications by Year
in descending order

Version: 2024-02-01

172 papers	12,549 citations	28242 55 h-index	24232 110 g-index
175 all docs	175 docs citations	175 times ranked	7564 citing authors

#	Article	IF	Citations
1	A simple empirical N-body potential for transition metals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1984, 50, 45-55.	0.7	2,878
2	SimpleN-body potentials for the noble metals and nickel. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1987, 56, 735-756.	0.7	558
3	The theory of metal - ceramic interfaces. Journal of Physics Condensed Matter, 1996, 8, 5811-5836.	0.7	490
4	The tight-binding bond model. Journal of Physics C: Solid State Physics, 1988, 21, 35-66.	1.5	422
5	Long range interactions in nanoscale science. Reviews of Modern Physics, 2010, 82, 1887-1944.	16.4	359
6	A stabilization mechanism of zirconia based on oxygen vacancies only. Acta Materialia, 2002, 50, 5171-5178.	3.8	330
7	Theory of lattice contraction at aluminium surfaces. Journal of Physics F: Metal Physics, 1974, 4, L37-L41.	1.6	305
8	The influence of grain boundary inclination on the structure and energy of Ïƒ = 3 grain boundaries in copper. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1992, 66, 991-1016.	0.7	193
9	Supercell size scaling of density functional theory formation energies of charged defects. Physical Review B, 2009, 79, .	1.1	180
10	Thermal excitation of electrons in energetic displacement cascades. Physical Review B, 1991, 44, 567-574.	1.1	177
11	Semi-empirical calculation of solid surface tensions in body-centred cubic transition metals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1986, 54, 301-315.	0.7	176
12	First-Principles Calculations of the Ideal Cleavage Energy of Bulk Niobium(111)/Î±-Alumina(0001) Interfaces. Physical Review Letters, 1999, 82, 1510-1513.	2.9	174
13	Bismuth embrittlement of copper is an atomic size effect. Nature, 2004, 432, 1008-1011.	13.7	174
14	Magnetism and thermodynamics of defect-free Fe-Cr alloys. Physical Review B, 2006, 74, .	1.1	174
15	Equilibrium and adhesion of Nb/sapphire: The effect of oxygen partial pressure. Physical Review B, 2000, 62, 4698-4706.	1.1	162
16	Theoretical prediction and direct observation of the 9Rstructure in Ag. Physical Review Letters, 1992, 69, 620-623.	2.9	157
17	SrTiO3(001)(2Ã—1)reconstructions:â€ƒFirst-principles calculations of surface energy and atomic structure compared with scanning tunneling microscopy images. Physical Review B, 2004, 70, .	1.1	154
18	On the growth of Al2O3 scales. Acta Materialia, 2013, 61, 6670-6683.	3.8	140

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19	Crystal Structures of Zirconia from First Principles and Self-Consistent Tight Binding. Physical Review Letters, 1998, 81, 5149-5152.	2.9	132
20	Irradiation creep models â€" an overview. Journal of Nuclear Materials, 1988, 159, 257-285.	1.3	129
21	THE OXIDATION OF NIAL: What Can We Learn from Ab Initio Calculations?. Annual Review of Materials Research, 2005, 35, 167-207.	4.3	129
22	Structural and chemical embrittlement of grain boundaries by impurities: A general theory and first-principles calculations for copper. Physical Review B, 2006, 74, .	1.1	127
23	Ab initio calculations on the Al2O3(0001) surface. Faraday Discussions, 1999, 114, 33-43.	1.6	124
24	The energy and elastic constants of simple metals in terms of pairwise interactions. Journal of Physics F: Metal Physics, 1974, 4, 1645-1656.	1.6	120
25	Validity of the second moment tight-binding model. Journal of Physics F: Metal Physics, 1988, 18, L153-L157.	1.6	120
26	Prediction of high-temperature point defect formation in TiO2 from combined ab initio and thermodynamic calculations. Acta Materialia, 2007, 55, 4325-4337.	3.8	120
27	The treatment of electronic excitations in atomistic models of radiation damage in metals. Reports on Progress in Physics, 2010, 73, 116501.	8.1	109
28	Metal-ceramic cohesion and the image interaction. Acta Metallurgica Et Materialia, 1992, 40, S25-S37.	1.9	106
29	Point defects and chemical potentials in ordered alloys. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1998, 77, 447-464.	0.7	101
30	Atom probe tomography analysis of the distribution of rhenium in nickel alloys. Acta Materialia, 2010, 58, 931-942.	3.8	101
31	Surface structure and water adsorption on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Fe</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mn>111</mml:mn> Spin-density functional theory and on-site Coulomb interactions. Physical Review B, 2008, 77, .	1.1	96
32	The Harris functional applied to surface and vacancy formation energies in aluminium. Journal of Physics Condensed Matter, 1990, 2, 331-342.	0.7	93
33	Improved method of calculatingab initiohigh-temperature thermodynamic properties with application to ZrC. Physical Review B, 2015, 91, .	1.1	86
34	Solid-liquid interface free energy through metadynamics simulations. Physical Review B, 2010, 81, .	1.1	84
35	Relative energetics and structural properties of zirconia using a self-consistent tight-binding model. Physical Review B, 2000, 61, 6617-6630.	1.1	82
36	Atomistic study of structural correlations at a liquidâ€"solid interface. Computational Materials Science, 2002, 24, 443-452.	1.4	79

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37	On the possibility of rhenium clustering in nickel-based superalloys. Acta Materialia, 2012, 60, 2866-2872.	3.8	78
38	Vacancy formation energies and linear screening theory. Journal of Physics F: Metal Physics, 1976, 6, 483-498.	1.6	75
39	The interaction of a point charge with an aluminium (111) surface. Surface Science, 1991, 241, 61-72.	0.8	73
40	First-Principles Approach to Model Electrochemical Reactions: Understanding the Fundamental Mechanisms behind Mg Corrosion. Physical Review Letters, 2018, 120, 246801.	2.9	71
41	Vacancy formation volumes in simple metals. Journal of Physics F: Metal Physics, 1976, 6, 965-978.	1.6	70
42	Transferable atomistic model to describe the energetics of zirconia. Physical Review B, 1996, 54, 9147-9161.	1.1	70
43	Interatomic potentials for strontium titanate: An assessment of their transferability and comparison with density functional theory. Physical Review B, 2008, 78, .	1.1	70
44	Surface Stoichiometry and the Initial Oxidation of NiAl(110). Physical Review Letters, 2000, 85, 610-613.	2.9	68
45	Interatomic Forces and Phonon Anomalies in bcc3dTransition Metals. Physical Review Letters, 1984, 52, 291-294.	2.9	67
46	Ab initioatomistic simulation of the strength of defective aluminum and tests of empirical force models. Physical Review B, 1995, 52, 15191-15207.	1.1	66
47	A critique of rhenium clustering in Niâ€“Re alloys using extended X-ray absorption spectroscopy. Acta Materialia, 2008, 56, 2669-2675.	3.8	65
48	First-Principles Calculations for Niobium Atoms on a Sapphire Surface. Journal of the American Ceramic Society, 1994, 77, 431-436.	1.9	64
49	Free energy and molecular dynamics calculations for the cubic-tetragonal phase transition in zirconia. Physical Review B, 2001, 63, .	1.1	64
50	Interatomic forces in transition metals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1988, 58, 143-163.	0.7	63
51	Transferable model for the atomistic simulation ofAl2O3. Physical Review B, 1996, 54, 15683-15689.	1.1	61
52	Perspectives on point defect thermodynamics. Physica Status Solidi (B): Basic Research, 2014, 251, 97-129.	0.7	58
53	Accessing the Excess: An Atomistic Approach to Excesses at Planar Defects and Dislocations in Ordered Compounds. Physica Status Solidi A, 1998, 166, 397-416.	1.7	57
54	Prediction and Observation of the bcc Structure in Pure Copper at aÎ£3 Grain Boundary. Physical Review Letters, 1995, 75, 2160-2163.	2.9	56

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55	Ordering at Solid-Liquid Interfaces Between Dissimilar Materials. Journal of Materials Science, 2001, 9, 175-181.	1.2	55
56	The diffusion of doxorubicin drug molecules in silica nanoslits is non-Gaussian, intermittent and anticorrelated. Physical Chemistry Chemical Physics, 2020, 22, 27955-27965.	1.3	55
57	A calculation of elastic constants of ferromagnetic iron at finite temperatures. Journal of Physics F: Metal Physics, 1985, 15, 19-34.	1.6	53
58	First-principles study of the atomistic and electronic structure of the niobium--alumina (0001) interface. Philosophical Magazine Letters, 1996, 73, 377-384.	0.5	53
59	Effect of relaxation on the oxygenK-edge electron energy-loss near-edge structure in yttria-stabilized zirconia. Physical Review B, 2000, 62, 14728-14735.	1.1	53
60	Analytic bond-order potentials for multicomponent systems. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2004, 365, 2-13.	2.6	53
61	Theoretical and experimental investigations of structures and energies of Î£ = 3, [112] tilt grain boundaries in copper. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1998, 77, 1161-1184.	0.7	52
62	Electron energy-loss near-edge shape as a probe to investigate the stabilization of yttria-stabilized zirconia. Physical Review B, 2002, 65, .	1.1	52
63	Plasmonic ELISA for the detection of gp120 at ultralow concentrations with the naked eye. Nanoscale, 2014, 6, 9559-9562.	2.8	52
64	The Band Structure of Polycrystalline Al₂O₃ and Its Influence on Transport Phenomena. Journal of the American Ceramic Society, 2016, 99, 733-747.	1.9	51
65	Anomalous diffusion along metal/ceramic interfaces. Nature Communications, 2018, 9, 5251.	5.8	51
66	Electronic damping of atomic dynamics in irradiation damage of metals. Journal of Physics Condensed Matter, 2007, 19, 436209.	0.7	50
67	Atomistic and electronic structure of Al/MgAl2O4and Ag/MgAl2O4interfaces. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2001, 81, 927-955.	0.7	49
68	Theoretical and experimental analysis of near Î£3 (211) boundaries in silver. Acta Metallurgica Et Materialia, 1994, 42, 3555-3567.	1.9	47
69	The Structure of Grain Boundaries in Strontium Titanate: Theory, Simulation, and Electron Microscopy. Annual Review of Materials Research, 2010, 40, 557-599.	4.3	47
70	Insight into gallium behavior in aluminum grain boundaries from calculation on Î£=11 (113) boundary. Acta Materialia, 2000, 48, 3623-3632.	3.8	46
71	Sputtering of gold foils in a high voltage electron microscope A comparison of theory and experiment. Philosophical Magazine and Journal, 1977, 35, 693-714.	1.8	44
72	Interstitials in FeCr alloys studied by density functional theory. Physical Review B, 2007, 76, .	1.1	44

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73	The interaction of a point charge with a metal surface: theory and calculations for (111), (100) and (110) aluminium surfaces. Journal of Physics Condensed Matter, 1995, 7, 2001-2019.	0.7	42
74	A comparison of methods for calculating tight-binding bond energies. Journal of Physics F: Metal Physics, 1988, 18, 693-718.	1.6	40
75	Magnetic tight binding and the iron-chromium enthalpy anomaly. Physical Review B, 2008, 77, .	1.1	39
76	Ab initio calculations of metal/ceramic interfaces: what have we learned, what can we learn?. Scripta Materialia, 1995, 6, 145-155.	0.5	35
77	The structure of special grain boundaries in Î±-Al2O3. Journal of Physics and Chemistry of Solids, 1994, 55, 1067-1082.	1.9	34
78	Bond-order potentials through the ages. Progress in Materials Science, 2007, 52, 133-153.	16.0	34
79	Why TiC(111) is observed to be Ti terminated. Surface Science, 1996, 348, 49-54.	0.8	33
80	Energetic and kinetic aspects of the faceting transformation of a Î£3 grain boundary in Cu. Acta Metallurgica Et Materialia, 1993, 41, 2163-2171.	1.9	32
81	Energetics of charged point defects in rutile TiO2 by density functional theory. Acta Materialia, 2009, 57, 5882-5891.	3.8	32
82	Determination of the Atomistic Structure of the â^'3 (111) Twin Boundary in NiAl. Materials Science Forum, 1996, 207-209, 245-248.	0.3	30
83	The energy of helium filled platelets and bubbles in molybdenum. Radiation Effects, 1983, 78, 121-132.	0.4	29
84	Pressure-Induced Isostructural Phase Transition in Al-Rich NiAl Alloys. Physical Review Letters, 1999, 83, 979-982.	2.9	29
85	A physically transparent and transferable compressible ion model for oxides. Journal of Chemical Physics, 2001, 114, 4406.	1.2	29
86	MEAMfit: A reference-free modified embedded atom method (RF-MEAM) energy and force-fitting code. Computer Physics Communications, 2015, 196, 439-445.	3.0	29
87	Electronic structures and phonon free energies of LaCoO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>using hybrid-exchange density functional theory. Physical Review B, 2013, 87, .	1.1	28
88	Surface energy and the early stages of oxidation of NiAl(110). Computer Physics Communications, 2001, 137, 174-194.	3.0	27
89	Oxygen vacancy formation energies in Sr-doped complex perovskites: ab initio thermodynamic study. Solid State Ionics, 2014, 254, 11-16.	1.3	26
90	A Density Functional Study of Interactions at the Metalâ€“Ceramic Interfaces Al/MgAl2O4 and Ag/MgAl2O4. Physica Status Solidi A, 1998, 166, 417-428.	1.7	25

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91	Bond energies and defect forces around a vacancy in BCC transition metals. Journal of Physics F: Metal Physics, 1987, 17, L273-L281.	1.6	24
92	Stability of Sr adatom model structures for SrTiO3(001) surface reconstructions. Journal of Physics Condensed Matter, 2005, 17, L223-L230.	0.7	24
93	Structural and electronic properties of Î£7 grain boundaries in Î±-Al2O3. Acta Materialia, 2015, 99, 16-28.	3.8	24
94	A simple theory of some phase transitions. Journal of Physics F: Metal Physics, 1974, 4, 960-968.	1.6	23
95	Plutonium redistribution in mixed oxide (U, Pu)O2 nuclear fuel elements. Journal of Nuclear Materials, 1978, 75, 193-200.	1.3	23
96	Atomistic study of ordinary screw dislocations in single-phase and lamellar Î³-TiAl. Philosophical Magazine, 2007, 87, 1795-1809.	0.7	23
97	The role of ceramic and glass science research in meeting societal challenges: Report from an ‹scp›NSF‹/scp›â€sponsored workshop. Journal of the American Ceramic Society, 2017, 100, 1777-1803.	1.9	23
98	Heat of transport in solids. III. Computer simulation of vacancy in an FCC crystal. Journal of Physics C: Solid State Physics, 1978, 11, 4469-4483.	1.5	22
99	Defect energies and linear screening theory in simple metals. Journal of Physics F: Metal Physics, 1975, 5, 2227-2240.	1.6	21
100	Ab initio computational study of Ga in an Al grain boundary. Philosophical Magazine Letters, 1997, 76, 281-288.	0.5	21
101	Structure of multilayer ZrO2/SrTiO3. Journal of Materials Science, 2012, 47, 1631-1640.	1.7	21
102	Phonon softening in ferromagnetic BCC iron. Journal of Physics F: Metal Physics, 1987, 17, 2049-2055.	1.6	20
103	The Î±-alumina(0001)surface: relaxations and dynamics from shell model and density functional theory. Journal of the European Ceramic Society, 2003, 23, 2729-2735.	2.8	20
104	Interatomic forces in materials. Progress in Materials Science, 2004, 49, 1-18.	16.0	19
105	Atomic-scale characterization of theSrTiO3Î£3(112)[1Â¯10]grain boundary. Physical Review B, 2010, 81, .	1.1	18
106	Representations of the local atomic density. Journal of Physics Condensed Matter, 1998, 10, 7983-7993.	0.7	16
107	The temperature dependence of the Debye-Waller factors of B2 NiAl. Philosophical Magazine Letters, 1996, 73, 137-144.	0.5	15
108	Ab initiotransmission electron microscopy image simulations of coherentAgâ¯'MgOinterfaces. Physical Review B, 2004, 70, .	1.1	15

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109	The challenges of hydrogen and metals. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20170198.	1.6	15
110	Theory of vacancy formation volume. Journal of Physics F: Metal Physics, 1977, 7, 1999-2010.	1.6	14
111	Migration mechanisms of a faceted grain boundary. Physical Review Materials, 2018, 2, .	0.9	14
112	The rÃ1e of the interface in determining the orientation of solid rare gas bubbles in metals. Acta Metallurgica, 1987, 35, 2543-2547.	2.1	13
113	Energies of defects in ordered alloys: dislocation core energies in NiAl. Acta Materialia, 1998, 46, 919-926.	3.8	13
114	Atomistic force field for alumina fit to density functional theory. Journal of Chemical Physics, 2013, 139, 204704.	1.2	13
115	Crack-Tip Blunting Versus Cleavage Extension. , 1983, , 1047-1051.		13
116	Observations and theory of thermally-induced helium bubble shrinkage in gold. Journal of Nuclear Materials, 1989, 168, 19-23.	1.3	12
117	Correlated electron-ion dynamics in metallic systems. Computational Materials Science, 2008, 44, 16-20.	1.4	12
118	Ab initiobased method to study structural phase transitions in dynamically unstable crystals, with new insights on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math>to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ï‰</mml:mi></mml:math>transformation in titanium. Physical Review B, 2019, 100, .	1.1	12
119	A theory of irradiation and thermal creep by dislocation climb. Journal of Nuclear Materials, 1981, 104, 1263-1267.	1.3	11
120	Dynamics and free energy of Â-alumina (0001) surfaces: I. Semi-empirical model. Journal of Physics Condensed Matter, 2002, 14, 7797-7810.	0.7	11
121	Electrostatic and Entropic Interactions between Parallel Interfaces Separated by a Glassy Film. Journal of the American Ceramic Society, 2002, 85, 2562-2568.	1.9	11
122	Atomistic Simulation of Grain Boundaries in Alumina. Materials Science Forum, 1996, 207-209, 225-228.	0.3	10
123	An Isothermal-Isobaric Langevin Thermostat for Simulating Nanoparticles under Pressure: Application to Au Clusters. ChemPhysChem, 2005, 6, 1848-1852.	1.0	10
124	Quantum mechanical simulations of electronic stopping in metals. Nuclear Instruments & Methods in Physics Research B, 2011, 269, 1640-1645.	0.6	10
125	Concepts for simulating and understanding materials at the atomic scale. MRS Bulletin, 2012, 37, 477-484.	1.7	10
126	Spontaneous Frenkel pair formation in zirconium carbide. Physical Review B, 2018, 98, .	1.1	10

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127	Fast anharmonic free energy method with an application to vacancies in ZrC. Physical Review B, 2019, 100, .	1.1	10
128	Point defects and chemical potentials in ordered alloys. , 0, .		10
129	Ab Initio Study of Electronic and Geometric Structures of Metal/Ceramic Heterophase Boundaries. Materials Research Society Symposia Proceedings, 1997, 492, 97.	0.1	8
130	Al-oxynitride interfacial layer investigations for Pr_XO_Yon SiC and Si. Journal of Physics: Conference Series, 2008, 94, 012004.	0.3	8
131	The movement of lenticular pores in mixed oxide (U, Pu) O2 nuclear fuel elements. Journal of Nuclear Materials, 1978, 75, 115-124.	1.3	7
132	First principles investigation of polarisation at interfaces in multilayered strontium titanate. Journal of Physics: Conference Series, 2008, 94, 012005.	0.3	6
133	Understanding adhesion between metal and oxide. Materials at High Temperatures, 1994, 12, 189-194.	0.5	5
134	Comment on â€œMetal-Ceramic Adhesion and the Harris Functionalâ€• Physical Review Letters, 1995, 74, 3083-3083.	2.9	5
135	Self-Consistent Tight-Binding Approximation Including Polarisable Ions. Materials Research Society Symposia Proceedings, 1997, 491, 265.	0.1	5
136	Solid-liquid phase equilibria from free-energy perturbation calculations. Physical Review B, 2008, 78, .	1.1	5
137	Changes in macroscopic behaviour through segregation in niobium doped strontium titanate. Journal of Physics: Conference Series, 2008, 94, 012015.	0.3	5
138	Stability of Zr-Al-C and Ti-Al-C MAX phases: A theoretical study. Physical Review Materials, 2021, 5, .	0.9	5
139	Grand canonical approach to modeling hydrogen trapping at vacancies in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â^’</mml:mtext><mml:mi>Fe</mml:mi> Physical Review Materials, 2020, 4, .		5
140	The theory of distorted structures in the Cd-Mg and In-Tl alloy systems. Journal of Physics F: Metal Physics, 1974, 4, 969-980.	1.6	4
141	Improved representation of metallic bonding in atomistic simulations. Philosophical Magazine Letters, 1996, 73, 39-44.	0.5	4
142	Studies of grain orientations and grain boundaries in polycrystalline SrTiO3. Journal of Physics: Conference Series, 2008, 94, 012008.	0.3	4
143	Calculating Grain Boundary Energies and Other Defect Energies in Ordered Alloys. , 1997, , 339-347.		4
144	Vacancy formation energies and volumes in simple metals. Journal of Nuclear Materials, 1978, 69-70, 638-640.	1.3	3

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145	Simulation on all length scales. Physics World, 1993, 6, 37-43.	0.0	3
146	A model for time-dependent grain boundary diffusion of ions and electrons through a film or scale, with an application to alumina. Acta Materialia, 2017, 132, 503-516.	3.8	3
147	Point Defects in NiAl Alloys Under Pressure. , 2000, , 439-454.		3
148	A theory of peaks in the time-of-flight spectrum of gold atoms sputtered from a (100) surface. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1981, 43, 1321-1344.	0.7	2
149	First Principles Calculations for Metal/Ceramic Interfaces. Materials Research Society Symposia Proceedings, 1994, 357, 427.	0.1	2
150	Calculating and Understanding the Structure of Interfaces. Materials Science Forum, 1996, 207-209, 35-46.	0.3	2
151	Bi_{3.25}La_{0.75}Ti₃O₁₂films on La₂Ti₂O₇thin films prepared by chemical solution deposition. Journal of Physics: Conference Series, 2008, 94, 012014.	0.3	2
152	Effect of surface orientation on intrinsic island formation on SrTiO₃surfaces. Journal of Physics: Conference Series, 2008, 94, 012013.	0.3	2
153	Dielectric properties of pure and Nb-doped SrTiO₃surfaces: a reflection electron energy loss spectroscopy study. Journal of Physics: Conference Series, 2008, 94, 012010.	0.3	2
154	Aiding the Design of Radiation Resistant Materials with Multiphysics Simulations of Damage Processes. Materials Research Society Symposia Proceedings, 2009, 1229, 30601.	0.1	2
155	New methods for calculating the free energy of charged defects in solid electrolytes. Journal of Physics Condensed Matter, 2013, 25, 395001.	0.7	2
156	Structure and ionic diffusivity in an yttria-stabilised zirconia/strontium titanate multilayer. Acta Materialia, 2017, 129, 388-397.	3.8	2
157	Response Functions and Interatomic Forces. Springer Series in Solid-state Sciences, 1987, , 120-131.	0.3	2
158	Interatomic Forces and the Simulation of Cracks. , 1987, , 177-195.		2
159	Instability of the rate equations for creep coupled to swelling. Journal of Nuclear Materials, 1985, 132, 277-283.	1.3	1
160	Prediction of the BCC Structure in a Cu â^'3-84Â° <211> Tilt Grain Boundary and Its Confirmation by HRTEM. Materials Science Forum, 1996, 207-209, 337-340.	0.3	1
161	The use of XANES and ELNES for the Characterisation of Stabilised Zirconia. Materials Research Society Symposia Proceedings, 2001, 699, 821.	0.1	1
162	A Density Functional Study of Interactions at the Metalâ€“Ceramic Interfaces Al/MgAl2O4 and Ag/MgAl2O4. Physica Status Solidi A, 1998, 166, 417-428.	1.7	1

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163	Atomistic and electronic structure of Al/MgAl2O4 and Ag/MgAl2O4 interfaces. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2001, 81, 927-955.	0.7	1
164	Diffusion of oxygen in Mg-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> : The corundum conundrum explained. Physical Review Materials, 2022, 6, .	0.9	1
165	Ab Initio and Model Calculations on Different Phases of Zirconia. Materials Research Society Symposia Proceedings, 1995, 408, 321.	0.1	0
166	A Coupled Compressible and Polarizable Ionic Model Applied to Oxide Crystal Structures. Materials Research Society Symposia Proceedings, 1998, 547, 197.	0.1	0
167	Simulation of a Grain Boundary in Zirconia. Materials Research Society Symposia Proceedings, 2000, 654, 151.	0.1	0
168	E-MRS 2002 Spring Meeting Symposium A: Atomic Scale Materials Design. Computational Materials Science, 2003, 27, xi-xii.	1.4	0
169	A faster way to relax interfaces in supercells. Journal of Physics Condensed Matter, 2004, 16, S2671-S2678.	0.7	0
170	Preface to the Special Section E-MRS MACAN. Journal of Materials Science, 2012, 47, 1603-1604.	1.7	0
171	Theoretical Aspects of Liquid Metal Embrittlement. , 1982, , 253-273.		0
172	Application of the Tight-Binding Bond Model. , 1989, , 369-380.		0