John H Harding

List of Publications by Year in descending order

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216 papers	8,041 citations	44069 48 h-index	62596 80 g-index
218 all docs	218 docs citations	218 times ranked	8104 citing authors

#	Article	IF	Citations
1	Significance of atomic-scale defects in flexible surfaces on local solvent and ion behaviour. Faraday Discussions, 2022, , .	3.2	1
2	Tuning the electrical conductivity of Rare Earth-doped BaTiO3 using Gd2O3 as an exemplar. Open Ceramics, 2022, 9, 100250.	2.0	3
3	Evaluation of correlated studies using liquid cell and cryoâ€transmission electron microscopy: Hydration of calcium sulphate and the phase transformation pathways of bassanite to gypsum. Journal of Microscopy, 2022, 288, 155-168.	1.8	7
4	A transferable force-field for alkali metal nitrates. Journal of Physics Communications, 2022, 6, 055011.	1.2	3
5	Multiple cascade radiation damage simulations of pyrochlore. Molecular Simulation, 2021, 47, 273-283.	2.0	2
6	The Role of Extracellular DNA in Microbial Attachment to Oxidized Silicon Surfaces in the Presence of Ca²⁺ and Na⁺. Langmuir, 2021, 37, 9838-9850.	3.5	6
7	The importance of the bacterial cell wall in uranium(<scp>vi</scp>) biosorption. Physical Chemistry Chemical Physics, 2021, 23, 1566-1576.	2.8	31
8	Using Metadynamics to Obtain the Free Energy Landscape for Cation Diffusion in Functional Ceramics: Dopant Distribution Control in Rare Earthâ€Doped BaTiO₃. Advanced Functional Materials, 2020, 30, 1905077.	14.9	13
9	Amino Acid and Oligopeptide Effects on Calcium Carbonate Solutions. Crystal Growth and Design, 2020, 20, 3077-3092.	3.0	19
10	The Analysis of Impedance Spectra for Coreâ€“Shell Microstructures: Why a Multiformalism Approach is Essential. Advanced Functional Materials, 2019, 29, 1904036.	14.9	13
11	Frontispiece: Ion Association in Lanthanide Chloride Solutions. Chemistry - A European Journal, 2019, 25, .	3.3	9
12	Simulation of Calcium Phosphate Prenucleation Clusters in Aqueous Solution: Association beyond Ion Pairing. Crystal Growth and Design, 2019, 19, 6422-6430.	3.0	41
13	Ion Association in Lanthanide Chloride Solutions. Chemistry - A European Journal, 2019, 25, 8725-8740.	3.3	5
14	Interaction of stable aggregates drives the precipitation of calcium phosphate in supersaturated solutions. CrystEngComm, 2019, 21, 6354-6364.	2.6	13
15	Electric field enhancement in ceramic capacitors due to interface amplitude roughness. Journal of the European Ceramic Society, 2019, 39, 1170-1177.	5.7	19
16	Simulation of Calcium Phosphate Species in Aqueous Solution: Force Field Derivation. Journal of Physical Chemistry B, 2018, 122, 1471-1483.	2.6	26
17	The Waterâ€“Amorphous Calcium Carbonate Interface and Its Interactions with Amino Acids. Crystal Growth and Design, 2017, 17, 5811-5822.	3.0	21
18	A new method for the generation of realistic atomistic models of siliceous MCM-41. Microporous and Mesoporous Materials, 2016, 228, 215-223.	4.4	14

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19	Tuning hardness in calcite by incorporation of amino acids. Nature Materials, 2016, 15, 903-910.	27.5	183
20	The role of extracellular DNA in uranium precipitation and biomineralisation. Physical Chemistry Chemical Physics, 2016, 18, 29101-29112.	2.8	17
21	Using simulation to understand the structure and properties of hydrated amorphous calcium carbonate. CrystEngComm, 2016, 18, 92-101.	2.6	19
22	Protein sequences bound to mineral surfaces persist into deep time. ELife, 2016, 5, .	6.0	176
23	Selective Ordering of Pertechnetate at the Interface between Amorphous Silica and Water: a Poisson Boltzmann Treatment. Materials Research Society Symposia Proceedings, 2015, 1744, 53-58.	0.1	0
24	Simulation of Impedance Spectra for Coreâ€“Shell Grain Structures Using FiniteÂElement Modeling. Journal of the American Ceramic Society, 2015, 98, 1925-1931.	3.8	20
25	How does an amorphous surface influence molecular binding? â€“ ovocleidin-17 and amorphous calcium carbonate. Physical Chemistry Chemical Physics, 2015, 17, 17494-17500.	2.8	13
26	Adsorption of poly acrylic acid onto the surface of calcite: an experimental and simulation study. Physical Chemistry Chemical Physics, 2015, 17, 27357-27365.	2.8	52
27	Order parameter and connectivity topology analysis of crystalline ceramics for nuclear waste immobilization. Journal of Physics Condensed Matter, 2014, 26, 485011.	1.8	6
28	Contact Resistance of Screen Printed Ag-Contacts to Si Emitters: Mathematical Modeling and Microstructural Characterization. Journal of the Electrochemical Society, 2014, 161, E3180-E3187.	2.9	2
29	Simulation of Impedance Spectra for a Full Threeâ€Dimensional Ceramic Microstructure Using a Finite Element Model. Journal of the American Ceramic Society, 2014, 97, 885-891.	3.8	23
30	A-Site Strain and Displacement in Ba1â€“xCaxTiO3 and Ba1â€“xSrxTiO3 and the Consequences for the Curie Temperature. Chemistry of Materials, 2014, 26, 6104-6112.	6.7	45
31	Effects of cationic substitution on structural defects in layered cathode materials LiNiO2. Journal of Materials Chemistry A, 2014, 2, 7988.	10.3	132
32	Oriented crystal growth on organic monolayers. CrystEngComm, 2014, 16, 1430-1438.	2.6	24
33	The Development of a Classical Force Field To Determine the Selectivity of an Aqueous Fe³⁺â€“EDA Complex for TcO₄^{â€“} and SO₄^{2â€“} Journal of Chemical Theory and Computation, 2014, 10, 3345-3353.	5.3	28
34	Entropy of Molecular Binding at Solvated Mineral Surfaces. Journal of Physical Chemistry C, 2014, 118, 1506-1514.	3.1	18
35	The interface of a-SiNx:H and Si: Linking the nano-scale structure to passivation quality. Solar Energy Materials and Solar Cells, 2014, 120, 311-316.	6.2	8
36	Energetics of Donorâ€Doping, Metal Vacancies, and Oxygenâ€Loss in Aâ€Site Rareâ€Earthâ€Doped BaTiO₃. Advanced Functional Materials, 2013, 23, 3925-3928.	14.9	70

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37	Phase stabilisation of hexagonal barium titanate doped with transition metals: A computational study. Journal of Solid State Chemistry, 2013, 200, 310-316.	2.9	24
38	A computational investigation of nickel (silicides) as potential contact layers for silicon photovoltaic cells. Journal of Physics Condensed Matter, 2013, 25, 395003.	1.8	10
39	Additions and corrections for Journal of Materials Chemistry C published in 2013. Journal of Materials Chemistry C, 2013, 1, 8222.	5.5	0
40	The application of a new potential model to the rare-earth doping of SrTiO3 and CaTiO3. Journal of Materials Chemistry C, 2013, 1, 1574.	5.5	48
41	Characterization of aâ€SiN_x:H layer: Bulk properties, interface with Si and solar cell efficiency. Physica Status Solidi (A) Applications and Materials Science, 2013, 210, 658-668.	1.8	10
42	Surface Selectivity of Calcite on Self-Assembled Monolayers. Journal of Physical Chemistry C, 2013, 117, 5154-5163.	3.1	14
43	The Influence of Aâ€Site Rare Earth Ion Size in Controlling the Curie Temperature of Ba_{1 â^' x}RE_xTi_{1 â^' x/4}O₃. Advanced Functional Materials, 2013, 23, 491-495.	14.9	51
44	Stoichiometrically graded SiNx for improved surface passivation in high performance solar cells. Journal of Applied Physics, 2012, 112, .	2.5	7
45	Nature of the hole states in Li-doped NiO. Physical Review B, 2012, 85, .	3.2	45
46	First-principles study of intrinsic point defects in hexagonal barium titanate. Journal of Applied Physics, 2012, 111, 094108.	2.5	18
47	Atomistic simulation of doping effects on growth and charge transport in Si/Ag interfaces in high-performance solar cells. Physical Review B, 2012, 86, .	3.2	11
48	Topological connectivity analysis of accumulated radiation damage from multiple molecular dynamics recoil cascades. Materials Research Society Symposia Proceedings, 2012, 1475, 577.	0.1	0
49	Examination of the properties of the interface of a-SiN_x:H/Si in crystalline silicon solar cells and its effect on cell efficiency. Materials Research Society Symposia Proceedings, 2012, 1423, 7.	0.1	3
50	The thermodynamics of calcite nucleation at organic interfaces: Classical vs. non-classical pathways. Faraday Discussions, 2012, 159, 509.	3.2	189
51	Novel potentials for modelling defect formation and oxygen vacancy migration in Gd2Ti2O7 and Gd2Zr2O7 pyrochlores. Journal of Materials Chemistry, 2012, 22, 4675.	6.7	36
52	Protein binding on stepped calcite surfaces: simulations of ovocleidin-17 on calcite {31.16} and {31.8}. Physical Chemistry Chemical Physics, 2012, 14, 7287.	2.8	29
53	Interface properties of a-SiNx:H/Si to improve surface passivation. Solar Energy Materials and Solar Cells, 2012, 106, 17-21.	6.2	20
54	Energetics of Ce and Pu incorporation into zirconolite waste-forms. Physical Chemistry Chemical Physics, 2011, 13, 13021.	2.8	14

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55	A new potential model for barium titanate and its implications for rare-earth doping. Journal of Materials Chemistry, 2011, 21, 4861.	6.7	81
56	Structural and electronic properties of silver/silicon interfaces and implications for solar cell performance. Physical Review B, 2011, 83, .	3.2	32
57	Simulations of Ovocleidin-17 Binding to Calcite Surfaces and Its Implications for Eggshell Formation. Journal of Physical Chemistry C, 2011, 115, 8175-8183.	3.1	64
58	Charge disproportionation and Jahn-Teller distortion in LiNiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>and NaNiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>: A density functional theory study. Physical Review B, 2011, 84, .	3.2	60
59	Sampling the structure of calcium carbonate nanoparticles with metadynamics. Journal of Chemical Physics, 2011, 134, 044703.	3.0	41
60	An atomistic study into the defect chemistry of hexagonal barium titanate. Journal of Applied Physics, 2011, 109, 084102.	2.5	29
61	Molecular dynamics studies of the bonding properties of amorphous silicon nitride coatings on crystalline silicon. Journal of Applied Physics, 2011, 110, .	2.5	14
62	Structural Control of Crystal Nuclei by an Eggshell Protein. Angewandte Chemie - International Edition, 2010, 49, 5135-5137.	13.8	100
63	EXAFS and Raman scattering studies of Y and Zr doped nano-crystalline tin oxide. Journal of Physics: Conference Series, 2010, 249, 012054.	0.4	3
64	A demonstration of the inhomogeneity of the local dielectric response of proteins by molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 235103.	3.0	32
65	Molecular dynamics simulations of peptides on calcite surface. Molecular Simulation, 2009, 35, 547-553.	2.0	27
66	Invited review: Mesoscopic modelling: Materials at the appropriate scale. Materials Science and Technology, 2009, 25, 460-465.	1.6	4
67	Interactions of Organic Molecules with Calcite and Magnesite Surfaces. Journal of Physical Chemistry C, 2009, 113, 3666-3673.	3.1	55
68	Ultrathin oxide films and heterojunctions: CaO layers on BaO and SrO. Physical Chemistry Chemical Physics, 2009, 11, 3217.	2.8	4
69	Metadynamics simulations of calcite crystallization on self-assembled monolayers. Journal of Chemical Physics, 2009, 131, 094703.	3.0	40
70	Physics of Nanomechanical Biosensing on Cantilever Arrays. Advanced Materials, 2008, 20, 3848-3853.	21.0	53
71	Computational Techniques at the Organicâ"Inorganic Interface in Biomineralization. Chemical Reviews, 2008, 108, 4823-4854.	47.7	113
72	Biological Control on Calcite Crystallization by Polysaccharides. Crystal Growth and Design, 2008, 8, 4066-4074.	3.0	110

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73	Simulations of Calcite Crystallization on Self-Assembled Monolayers. Langmuir, 2008, 24, 9607-9615.	3.5	32
74	Ultrathin oxide films: CaO layers on BaO and SrO. Materials Research Society Symposia Proceedings, 2008, 1148, 1.	0.1	1
75	Simulations of monosaccharide on calcite surfaces. Mineralogical Magazine, 2008, 72, 295-299.	1.4	9
76	A Theoretical Study of Ultra-Thin Films with the Wurtzite and Zinc Blende Structures. Materials Research Society Symposia Proceedings, 2007, 1035, 1.	0.1	0
77	New Forcefields for Modeling Biomineralization Processes. Journal of Physical Chemistry C, 2007, 111, 11943-11951.	3.1	119
78	The challenge of biominerals to simulations. Journal of Materials Chemistry, 2006, 16, 1105-1112.	6.7	69
79	Graphitic Nanofilms as Precursors to Wurtzite Films: Theory. Physical Review Letters, 2006, 96, 066102.	7.8	514
80	Nucleation and growth on defect sites: experimentâ€“theory comparison for Pd/MgO(001). Journal of Physics Condensed Matter, 2006, 18, S411-S427.	1.8	26
81	Correlation of Structural and Electronic Properties in a New Low-Dimensional Form of Mercury Telluride. Physical Review Letters, 2006, 96, 215501.	7.8	78
82	Atomistic simulations of surface diffusion and segregation in ceramics. Computational Materials Science, 2006, 36, 54-59.	3.0	7
83	Structural correlation of band-gap modifications induced in mercury telluride by dimensional constraint in single walled carbon nanotubes. Physica Status Solidi (B): Basic Research, 2006, 243, 3257-3262.	1.5	14
84	Thin films of wÃ¼rtzite materialsâ€”AlN vs. AlP. Journal of Crystal Growth, 2006, 294, 111-117.	1.5	6
85	Modelling of plasma particle interactions and coating growth for plasma spraying of hydroxyapatite. Surface and Coatings Technology, 2006, 200, 3757-3769.	4.8	58
86	Cohesion and polymorphism in solid rubidium chloride. Journal of Physics Condensed Matter, 2006, 18, 683-702.	1.8	8
87	The crystallisation of calcite clusters on self-assembled monolayers. Surface Science, 2005, 595, 151-156.	1.9	19
88	MgO addimer diffusion on MgO(100): A comparison ofab initioand empirical models. Physical Review B, 2005, 72, .	3.2	64
89	Surface diffusion and surface growth in nanofilms of mixed rocksalt oxides. Physical Chemistry Chemical Physics, 2005, 7, 1839.	2.8	14
90	Modeling the Properties of Self-Assembled Monolayers Terminated by Carboxylic Acids. Langmuir, 2005, 21, 3850-3857.	3.5	29

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91	Effect of Bicarbonate Ions on the Crystallization of Calcite on Self-Assembled Monolayers. Journal of Physical Chemistry B, 2005, 109, 5713-5718.	2.6	28
92	Growth of ZnO thin filmsâ€"experiment and theory. Journal of Materials Chemistry, 2005, 15, 139-148.	6.7	364
93	Novel exchange mechanisms in the surface diffusion of oxides. Journal of Physics Condensed Matter, 2004, 16, L187-L192.	1.8	15
94	Simulating surface diffusion and surface growth in ceramics. Dalton Transactions, 2004, , 3071.	3.3	4
95	Growth of Polar Crystal Surfaces on Ionized Organic Substrates. Langmuir, 2004, 20, 7637-7642.	3.5	50
96	Simulation of Organic Monolayers as Templates for the Nucleation of Calcite Crystals. Langmuir, 2004, 20, 7630-7636.	3.5	94
97	Short-Circuit Diffusion in Ceramics. Journal of Materials Science, 2003, 11, 81-90.	1.2	27
98	Experiment and Theory of Diffusion in Alumina. Journal of the American Ceramic Society, 2003, 86, 554-59.	3.8	85
99	Not too big, not too small: The appropriate scale. Nature Materials, 2003, 2, 77-83.	27.5	47
100	Selective nucleation and controlled growth: quantum dots on metal, insulator and semiconductor surfaces. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 311-329.	3.4	13
101	Atomistic Simulation of the Dissociative Adsorption of Water on Calcite Surfaces. Journal of Physical Chemistry B, 2003, 107, 7676-7682.	2.6	141
102	Shape control and applications of nanocrystals. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 241-257.	3.4	184
103	New synthetic routes for quantum dots. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 297-310.	3.4	40
104	Synthesis and selfâ€"assembly of colloidal nanoparticles. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 229-240.	3.4	77
105	Molecular dynamics simulations of the incorporation of Mg 2+ , Cd 2+ and Sr 2+ at calcite growth steps: Introduction of a SrCO 3 potential model. Molecular Simulation, 2002, 28, 573-589.	2.0	12
106	Control of inorganic morphologies by organic templates. Materials Research Society Symposia Proceedings, 2002, 735, 1151.	0.1	0
107	Simulating Oxide Interfaces and Heterointerfaces. Materials Research Society Symposia Proceedings, 2002, 751, 1.	0.1	0
108	Calcite and related materials: Growth and dissolution. Molecular Simulation, 2002, 28, 473-474.	2.0	0

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109	Modelling the interfaces between calcite crystals and Langmuir monolayers. Journal of Materials Chemistry, 2002, 12, 3419-3425.	6.7	46
110	Ca-induced surface reconstructions on TiO2(110) studied by scanning tunneling microscopy, reflection high-energy electron diffraction and atomistic simulation. Surface Science, 2001, 473, 151-157.	1.9	16
111	The surface structure of CeO2(001) single crystals studied by elevated temperature STM. Surface Science, 2001, 477, 17-24.	1.9	102
112	A theoretical study of lithium intercalation into V6O13â€"a combined classical, quantum mechanical approach. Physical Chemistry Chemical Physics, 2001, 3, 4052-4059.	2.8	25
113	Molecular Dynamics simulation of aqueous ZnC12solutions. Molecular Physics, 2001, 99, 825-833.	1.7	37
114	Simulation of grain-boundary diffusion in ceramics by kinetic Monte Carlo. Physical Review B, 2001, 63, .	3.2	20
115	A physically transparent and transferable compressible ion model for oxides. Journal of Chemical Physics, 2001, 114, 4406.	3.0	29
116	Nucleation and growth of supported metal clusters at defect sites on oxide and halide (001) surfaces. Journal of Crystal Growth, 2000, 211, 27-33.	1.5	59
117	Computer simulation of the reactive element effect in NiO grain boundaries. Acta Materialia, 2000, 48, 3039-3048.	7.9	20
118	Modelling of silver adhesion on MgO(100) surface with defects. Journal of Physics Condensed Matter, 2000, 12, 55-66.	1.8	19
119	A computational study of the high voltage LixCoyMn4-yO8 cathode material. Physical Chemistry Chemical Physics, 2000, 2, 3841-3846.	2.8	16
120	Calculated cell discharge curve for lithium batteries with a V2O5 cathode. Journal of Materials Chemistry, 2000, 10, 239-240.	6.7	20
121	Atomistic simulation methodologies for modelling the nucleation, growth and structure of interfaces. Journal of Materials Chemistry, 2000, 10, 1315-1324.	6.7	24
122	Ordered structures of calcium oxide onTiO2(110)studied by STM and atomistic simulation. Physical Review B, 1999, 59, 9842-9845.	3.2	22
123	Computer simulation of general grain boundaries in rocksalt oxides. Physical Review B, 1999, 60, 2740-2746.	3.2	25
124	Simulations of surfaces and interfaces in MgO. Radiation Effects and Defects in Solids, 1999, 151, 299-304.	1.2	3
125	Formation of highly ordered Ca-overlayers on TiO2(110) surfaces studied by scanning tunneling microscopy and atomistic simulation. Applied Surface Science, 1999, 142, 174-176.	6.1	11
126	Molecular dynamics simulation of crystal dissolution from calcite steps. Physical Review B, 1999, 60, 13792-13799.	3.2	93

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127	The effect of impurities on vacancy migration at NiO grain boundaries. Radiation Effects and Defects in Solids, 1999, 151, 305-309.	1.2	0
128	Comparative theoretical study of the Agâ€“MgO (100) and (110) interfaces. Surface Science, 1999, 441, 373-383.	1.9	32
129	Lithium Intercalation into Vanadium Pentoxide:Â a Theoretical Study. Chemistry of Materials, 1999, 11, 1990-1998.	6.7	122
130	Nucleation and Growth of Supported Metal Clusters at Defect Sites on Mgo and NaCl (001) Surfaces: The Cases of Pd and Ag. Materials Research Society Symposia Proceedings, 1999, 570, 51.	0.1	5
131	Modelling the production and performance analysis of plasma-sprayed ceramic thermal barrier coatings. Archives of Computational Methods in Engineering, 1998, 5, 59-166.	10.2	17
132	Predicting nucleation and growth processes: Atomistic modeling of metal atoms on ionic substrates. Physical Review B, 1998, 57, 6715-6719.	3.2	26
133	Vibrational Pocket Modes: Predictions by the Embedded Crystallite Method and Their Experimental Observation. Physical Review Letters, 1998, 81, 3687-3690.	7.8	3
134	Simulation of the Growth of Heterostructures. Materials Research Society Symposia Proceedings, 1998, 529, 55.	0.1	0
135	Making the Connection Between Atomistic Modelling of Interfaces and Real Materials. , 1998, , 13-22.		0
136	The thermal conductivity of defective crystals. Journal of Chemical Physics, 1997, 106, 3681-3687.	3.0	17
137	Modelling oxygen vacancies at the Si(100)-SiO₂ interface. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1997, 75, 1435-1445.	0.6	8
138	Simulation Studies of Oxide Materials. Molecular Simulation, 1997, 20, 27-39.	2.0	4
139	Computer Simulation of Interfaces in Ceramics. Materials Research Society Symposia Proceedings, 1997, 492, 85.	0.1	1
140	Mesoscopic modelling. Current Opinion in Solid State and Materials Science, 1997, 2, 728-732.	11.5	2
141	Molecular dynamics simulations of compressible ions. Journal of Chemical Physics, 1996, 104, 8068-8081.	3.0	94
142	The Shell Model and Interatomic Potentials for Ceramics. MRS Bulletin, 1996, 21, 29-35.	3.5	28
143	A calculation of the structure and energy of theNb/Al 2 O 3 interface. Acta Materialia, 1996, 44, 3293-3298.	7.9	30
144	Modeling the deposition process of thermal barrier coatings. Journal of Thermal Spray Technology, 1995, 4, 34-40.	3.1	26

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146	A simulation of the NiO/Ag interface with point defects. Acta Metallurgica Et Materialia, 1995, 43, 1559-1568.	1.8	31
147	The stability of defects in the ceramic interfaces, and. Surface Science, 1995, 334, 170-178.	1.9	30
148	The meaning of the oxygen second-electron affinity and oxide potential models. Philosophical Magazine Letters, 1995, 71, 113-121.	1.2	70
149	Interionic potentials for oxides: Theory and applications. Radiation Effects and Defects in Solids, 1994, 129, 77-80.	1.2	0
150	Small-polaron hopping in Mott-insulating UO2. Journal of Physics Condensed Matter, 1994, 6, 4685-4698.	1.8	35
151	The cohesion of thorium dioxide. Journal of Physics Condensed Matter, 1994, 6, 6485-6496.	1.8	26
152	The polarizabilities and dispersion coefficients for ions in the solid group IV oxides. Journal of Physics Condensed Matter, 1994, 6, 10593-10606.	1.8	27
153	Effect of defects on the stability of heteroepitaxial ceramic interfaces studied by computer simulation. Physical Review B, 1994, 50, 14498-14505.	3.2	19
154	Interface stability and the growth of optical quality perovskites on MgO. Physical Review Letters, 1994, 72, 2741-2744.	7.8	132
155	The energies of point defects near metal/oxide interfaces. Journal of Applied Physics, 1994, 76, 2791-2798.	2.5	36
156	Accommodation of the misfit strain energy in the BaO(100)/MgO(100) heteroepitaxial ceramic interface using computer simulation techniques. Journal of Materials Chemistry, 1994, 4, 1883.	6.7	12
157	A Study of Thin Film YBa₂Cu₃O_{6.5}/MgO Interfaces Using a Near Coincidence Site Lattice Theory with Atomistic Simulation. Molecular Simulation, 1994, 12, 127-139.	2.0	8
158	Calculated defect formation energies as a function of distance from the BaO/MgO interface compared with image theory predictions. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1994, 69, 787-792.	0.6	7
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160	The effect of alloying elements on Zircaloy corrosion. Journal of Nuclear Materials, 1993, 202, 216-221.	2.7	18
161	Computer simulation of thin film heteroepitaxial ceramic interfaces using a near-coincidence-site lattice theory. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1993, 68, 565-573.	0.6	61
162	Atomistic modelling of metal-oxide interfaces with image interactions. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1993, 67, 865-882.	0.6	86

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163	Thermodynamic calculations of stannic oxide surfaces. European Physical Journal Special Topics, 1993, 03, C7-1971-C7-1974.	0.2	2
164	Atomistic modelling of the metal/oxide interface with image interactions. Acta Metallurgica Et Materialia, 1992, 40, S11-S16.	1.8	75
165	The stability of SnO2surfaces. Modelling and Simulation in Materials Science and Engineering, 1992, 1, 39-43.	2.0	74
166	A simple statistical model for grain growth in materials. Acta Metallurgica Et Materialia, 1991, 39, 2251-2254.	1.8	15
167	The V_kcentre in NaCl. Radiation Effects and Defects in Solids, 1991, 119-121, 27-32.	1.2	5
168	Interionic Potentials: A Users Guide. , 1991, , 159-182.		4
169	Computer simulation of plasma-sprayed coatings I. Coating deposition model. Surface and Coatings Technology, 1991, 48, 137-145.	4.8	50
170	Computer simulation of plasma-sprayed coatings II. Effective bulk properties and thermal stress calculations. Surface and Coatings Technology, 1991, 48, 147-154.	4.8	19
171	Defect parameters in the alkali halides. Radiation Effects and Defects in Solids, 1991, 119-121, 257-262.	1.2	1
172	Quadrupole terms in defect energies in transition metal oxides. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1990, 62, 487-497.	0.6	2
173	Simulation of Thermal Barrier Plasma-Sprayed Coatings. Materials Research Society Symposia Proceedings, 1990, 190, 221.	0.1	1
174	Computer modelling of the defect structure of non-stoichiometric binary transition metal oxides. Journal of Physics and Chemistry of Solids, 1990, 51, 477-506.	4.0	71
175	The prediction of correlation factors and motion energies for diffusion of transition metal ions in CoO and NiO. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1990, 62, 473-486.	0.6	3
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177	Computer simulation of defects in ionic solids. Reports on Progress in Physics, 1990, 53, 1403-1466.	20.1	161
178	The Practical Calculation of Interionic Potentials. Molecular Simulation, 1990, 4, 255-268.	2.0	12
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180	Calculation of the entropy of defect processes in ionic solids. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 351.	1.1	10

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181	DEFECTS AND TRANSPORT IN IONIC SOLIDS. Series on Directions in Condensed Matter Physics, 1989, , 107-168.	0.1	1
182	Defect structures and ionic transport in lithium oxide. Solid State Ionics, 1988, 28-30, 185-188.	2.7	55
183	The electrical impedance of single-crystal urania at elevated temperatures. Journal of Nuclear Materials, 1988, 154, 245-252.	2.7	13
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