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	Graphitic Nanofilms as Precursors to Wurtzite Films: Theory. Physical Review Letters, 2006, 96, 066102.	7.8	514
2	Growth of ZnO thin filmsâ€"experiment and theory. Journal of Materials Chemistry, 2005, 15, 139-148.	6.7	364
3	Dopant ion radius and ionic conductivity in cerium dioxide. Solid State Ionics, 1983, 8, 109-113.	2.7	274
4	The thermodynamics of calcite nucleation at organic interfaces: Classical vs. non-classical pathways. Faraday Discussions, 2012, 159, 509.	3.2	189
5	Shape control and applications of nanocrystals. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 241-257.	3.4	184
6	Tuning hardness in calcite by incorporation of amino acids. Nature Materials, 2016, 15, 903-910.	27.5	183
7	Protein sequences bound to mineral surfaces persist into deep time. ELife, 2016, 5, .	6.0	176
8	Computer simulation of defects in ionic solids. Reports on Progress in Physics, 1990, 53, 1403-1466.	20.1	161
9	Atomistic Simulation of the Dissociative Adsorption of Water on Calcite Surfaces. Journal of Physical Chemistry B, 2003, 107, 7676-7682.	2.6	141
10	The calculation of defect parameters in UO₂. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1986, 53, 27-50.	0.6	135
11	Interface stability and the growth of optical quality perovskites on MgO. Physical Review Letters, 1994, 72, 2741-2744.	7.8	132
12	Effects of cationic substitution on structural defects in layered cathode materials LiNiO2. Journal of Materials Chemistry A, 2014, 2, 7988.	10.3	132
13	Lithium Intercalation into Vanadium Pentoxide:Â a Theoretical Study. Chemistry of Materials, 1999, 11, 1990-1998.	6.7	122
14	New Forcefields for Modeling Biomineralization Processes. Journal of Physical Chemistry C, 2007, 111, 11943-11951.	3.1	119
15	Computational Techniques at the Organicâ"Inorganic Interface in Biomineralization. Chemical Reviews, 2008, 108, 4823-4854.	47.7	113
16	Biological Control on Calcite Crystallization by Polysaccharides. Crystal Growth and Design, 2008, 8, 4066-4074.	3.0	110
17	A recommendation for the thermal conductivity of UO2. Journal of Nuclear Materials, 1989, 166, 223-226.	2.7	106
18	The surface structure of CeO2(001) single crystals studied by elevated temperature STM. Surface Science, 2001, 477, 17-24.	1.9	102

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19	Structural Control of Crystal Nuclei by an Eggshell Protein. Angewandte Chemie - International Edition, 2010, 49, 5135-5137.	13.8	100
20	Molecular dynamics simulations of compressible ions. Journal of Chemical Physics, 1996, 104, 8068-8081.	3.0	94
21	Simulation of Organic Monolayers as Templates for the Nucleation of Calcite Crystals. Langmuir, 2004, 20, 7630-7636.	3.5	94
22	Molecular dynamics simulation of crystal dissolution from calcite steps. Physical Review B, 1999, 60, 13792-13799.	3.2	93
23	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
24	Experiment and Theory of Diffusion in Alumina. Journal of the American Ceramic Society, 2003, 86, 554-59.	3.8	85
25	A new potential model for barium titanate and its implications for rare-earth doping. Journal of Materials Chemistry, 2011, 21, 4861.	6.7	81
26	Correlation of Structural and Electronic Properties in a New Low-Dimensional Form of Mercury Telluride. Physical Review Letters, 2006, 96, 215501.	7.8	78
27	Synthesis and selfâ€“assembly of colloidal nanoparticles. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 229-240.	3.4	77
28	Atomistic modelling of the metal/oxide interface with image interactions. Acta Metallurgica Et Materialia, 1992, 40, S11-S16.	1.8	75
29	Hartree-Fock cluster computations of defect and perfect ionic crystal properties. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1985, 131, 151-156.	0.9	74
30	The stability of SnO2surfaces. Modelling and Simulation in Materials Science and Engineering, 1992, 1, 39-43.	2.0	74
31	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
32	The meaning of the oxygen second-electron affinity and oxide potential models. Philosophical Magazine Letters, 1995, 71, 113-121.	1.2	70
33	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
34	The challenge of biominerals to simulations. Journal of Materials Chemistry, 2006, 16, 1105-1112.	6.7	69
35	Calculation of the free energy of defects in calcium fluoride. Physical Review B, 1985, 32, 6861-6872.	3.2	67
36	MgO addimer diffusion on MgO(100): A comparison ofab initioand empirical models. Physical Review B, 2005, 72, .	3.2	64

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37	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
38	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
39	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
40	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
41	Modelling of plasma particle interactions and coating growth for plasma spraying of hydroxyapatite. Surface and Coatings Technology, 2006, 200, 3757-3769.	4.8	58
42	Defect structures and ionic transport in lithium oxide. Solid State Ionics, 1988, 28-30, 185-188.	2.7	55
43	Interactions of Organic Molecules with Calcite and Magnesite Surfaces. Journal of Physical Chemistry C, 2009, 113, 3666-3673.	3.1	55
44	Physics of Nanomechanical Biosensing on Cantilever Arrays. Advanced Materials, 2008, 20, 3848-3853.	21.0	53
45	Thermodynamic properties of uranium dioxide: Electronic contributions to the specific heat. Journal of Nuclear Materials, 1980, 92, 73-78.	2.7	52
46	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
47	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
48	Computer simulation of plasma-sprayed coatings I. Coating deposition model. Surface and Coatings Technology, 1991, 48, 137-145.	4.8	50
49	Growth of Polar Crystal Surfaces on Ionized Organic Substrates. Langmuir, 2004, 20, 7637-7642.	3.5	50
50	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
51	Not too big, not too small: The appropriate scale. Nature Materials, 2003, 2, 77-83.	27.5	47
52	Calculations for electronic point defects with self-consistent lattice polarisation: the F+centre in MgO. Journal of Physics C: Solid State Physics, 1984, 17, 3401-3414.	1.5	46
53	Modelling the interfaces between calcite crystals and Langmuir monolayers. Journal of Materials Chemistry, 2002, 12, 3419-3425.	6.7	46
54	Nature of the hole states in Li-doped NiO. Physical Review B, 2012, 85, .	3.2	45

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55	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
56	Sampling the structure of calcium carbonate nanoparticles with metadynamics. Journal of Chemical Physics, 2011, 134, 044703.	3.0	41
57	Simulation of Calcium Phosphate Prenucleation Clusters in Aqueous Solution: Association beyond Ion Pairing. Crystal Growth and Design, 2019, 19, 6422-6430.	3.0	41
58	New synthetic routes for quantum dots. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 297-310.	3.4	40
59	Metadynamics simulations of calcite crystallization on self-assembled monolayers. Journal of Chemical Physics, 2009, 131, 094703.	3.0	40
60	Molecular Dynamics simulation of aqueous ZnC12solutions. Molecular Physics, 2001, 99, 825-833.	1.7	37
61	The energies of point defects near metal/oxide interfaces. Journal of Applied Physics, 1994, 76, 2791-2798.	2.5	36
62	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
63	Small-polaron hopping in Mott-insulating UO2. Journal of Physics Condensed Matter, 1994, 6, 4685-4698.	1.8	35
64	Conductivity and NMR study of ionic mobility in lithium oxide. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 1239.	1.7	33
65	Comparative theoretical study of the Agâ€“MgO (100) and (110) interfaces. Surface Science, 1999, 441, 373-383.	1.9	32
66	Simulations of Calcite Crystallization on Self-Assembled Monolayers. Langmuir, 2008, 24, 9607-9615.	3.5	32
67	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
68	Structural and electronic properties of silver/silicon interfaces and implications for solar cell performance. Physical Review B, 2011, 83, .	3.2	32
69	A simulation of the NiO/Ag interface with point defects. Acta Metallurgica Et Materialia, 1995, 43, 1559-1568.	1.8	31
70	The importance of the bacterial cell wall in uranium(<scp>vi</scp>) biosorption. Physical Chemistry Chemical Physics, 2021, 23, 1566-1576.	2.8	31
71	The stability of defects in the ceramic interfaces, and. Surface Science, 1995, 334, 170-178.	1.9	30
72	A calculation of the structure and energy of theNb/Al 2 O 3 interface. Acta Materialia, 1996, 44, 3293-3298.	7.9	30

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73	Vibrational entropies of defects in solids. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1981, 43, 705-713.	0.6	29
74	Entropy of segregation of isovalent impurity cations at the surface of an ionic crystal: MgO(100)Ca2+. Surface Science, 1986, 173, 439-454.	1.9	29
75	A calculation of defect Gibbs energies for silver chloride and silver bromide. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1987, 55, 481-498.	0.6	29
76	A physically transparent and transferable compressible ion model for oxides. Journal of Chemical Physics, 2001, 114, 4406.	3.0	29
77	Modeling the Properties of Self-Assembled Monolayers Terminated by Carboxylic Acids. Langmuir, 2005, 21, 3850-3857.	3.5	29
78	An atomistic study into the defect chemistry of hexagonal barium titanate. Journal of Applied Physics, 2011, 109, 084102.	2.5	29
79	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
80	The calculation of free energies of point defects in ionic crystals. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1985, 131, 13-26.	0.9	28
81	The Shell Model and Interatomic Potentials for Ceramics. MRS Bulletin, 1996, 21, 29-35.	3.5	28
82	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
83	The Development of a Classical Force Field To Determine the Selectivity of an Aqueous Fe³⁺â€“EDA Complex for TcO₄^{â€“} and SO₄^{2â€“}5.3 Journal of Chemical Theory and Computation, 2014, 10, 3345-3353.		28
84	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
85	Short-Circuit Diffusion in Ceramics. Journal of Materials Science, 2003, 11, 81-90.	1.2	27
86	Molecular dynamics simulations of peptides on calcite surface. Molecular Simulation, 2009, 35, 547-553.	2.0	27
87	Calculations of interionic potentials in oxides. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1985, 51, 119-125.	0.6	26
88	The cohesion of thorium dioxide. Journal of Physics Condensed Matter, 1994, 6, 6485-6496.	1.8	26
89	Modeling the deposition process of thermal barrier coatings. Journal of Thermal Spray Technology, 1995, 4, 34-40.	3.1	26
90	Predicting nucleation and growth processes: Atomistic modeling of metal atoms on ionic substrates. Physical Review B, 1998, 57, 6715-6719.	3.2	26

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91	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
92	Simulation of Calcium Phosphate Species in Aqueous Solution: Force Field Derivation. Journal of Physical Chemistry B, 2018, 122, 1471-1483.	2.6	26
93	Computer simulation of general grain boundaries in rocksalt oxides. Physical Review B, 1999, 60, 2740-2746.	3.2	25
94	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
95	Defect energies in ZnSe. Journal of Physics C: Solid State Physics, 1982, 15, 4649-4659.	1.5	24
96	Atomistic simulation methodologies for modelling the nucleation, growth and structure of interfaces. Journal of Materials Chemistry, 2000, 10, 1315-1324.	6.7	24
97	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
98	Oriented crystal growth on organic monolayers. CrystEngComm, 2014, 16, 1430-1438.	2.6	24
99	Calculation of defect migration rates by molecular dynamics simulation. Journal of Physics C: Solid State Physics, 1987, 20, 2331-2346.	1.5	23
100	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
101	Ordered structures of calcium oxide onTiO2(110)studied by STM and atomistic simulation. Physical Review B, 1999, 59, 9842-9845.	3.2	22
102	The Waterâ€“Amorphous Calcium Carbonate Interface and Its Interactions with Amino Acids. Crystal Growth and Design, 2017, 17, 5811-5822.	3.0	21
103	Computer simulation of the reactive element effect in NiO grain boundaries. Acta Materialia, 2000, 48, 3039-3048.	7.9	20
104	Calculated cell discharge curve for lithium batteries with a V2O5 cathode. Journal of Materials Chemistry, 2000, 10, 239-240.	6.7	20
105	Simulation of grain-boundary diffusion in ceramics by kinetic Monte Carlo. Physical Review B, 2001, 63, .	3.2	20
106	Interface properties of a-SiNx:H/Si to improve surface passivation. Solar Energy Materials and Solar Cells, 2012, 106, 17-21.	6.2	20
107	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
108	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

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109	Effect of defects on the stability of heteroepitaxial ceramic interfaces studied by computer simulation. Physical Review B, 1994, 50, 14498-14505.	3.2	19
110	Modelling of silver adhesion on MgO(100) surface with defects. Journal of Physics Condensed Matter, 2000, 12, 55-66.	1.8	19
111	The crystallisation of calcite clusters on self-assembled monolayers. Surface Science, 2005, 595, 151-156.	1.9	19
112	Using simulation to understand the structure and properties of hydrated amorphous calcium carbonate. CrystEngComm, 2016, 18, 92-101.	2.6	19
113	Electric field enhancement in ceramic capacitors due to interface amplitude roughness. Journal of the European Ceramic Society, 2019, 39, 1170-1177.	5.7	19
114	Amino Acid and Oligopeptide Effects on Calcium Carbonate Solutions. Crystal Growth and Design, 2020, 20, 3077-3092.	3.0	19
115	The effect of alloying elements on Zircaloy corrosion. Journal of Nuclear Materials, 1993, 202, 216-221.	2.7	18
116	First-principles study of intrinsic point defects in hexagonal barium titanate. Journal of Applied Physics, 2012, 111, 094108.	2.5	18
117	Entropy of Molecular Binding at Solvated Mineral Surfaces. Journal of Physical Chemistry C, 2014, 118, 1506-1514.	3.1	18
118	The thermal conductivity of defective crystals. Journal of Chemical Physics, 1997, 106, 3681-3687.	3.0	17
119	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
120	The role of extracellular DNA in uranium precipitation and biomineralisation. Physical Chemistry Chemical Physics, 2016, 18, 29101-29112.	2.8	17
121	The calculation of Hugoniots in ionic solids. Journal of Physics C: Solid State Physics, 1984, 17, 1179-1189.	1.5	16
122	A computational study of the high voltage LixCoyMn4-yO8 cathode material. Physical Chemistry Chemical Physics, 2000, 2, 3841-3846.	2.8	16
123	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
124	A simple statistical model for grain growth in materials. Acta Metallurgica Et Materialia, 1991, 39, 2251-2254.	1.8	15
125	Novel exchange mechanisms in the surface diffusion of oxides. Journal of Physics Condensed Matter, 2004, 16, L187-L192.	1.8	15
126	Vibrational modes of the Vkcentres in alkali halides. Journal of Physics C: Solid State Physics, 1980, 13, 3505-3510.	1.5	14

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127	Surface diffusion and surface growth in nanofilms of mixed rocksalt oxides. Physical Chemistry Chemical Physics, 2005, 7, 1839.	2.8	14
128	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
129	Energetics of Ce and Pu incorporation into zirconolite waste-forms. Physical Chemistry Chemical Physics, 2011, 13, 13021.	2.8	14
130	Molecular dynamics studies of the bonding properties of amorphous silicon nitride coatings on crystalline silicon. Journal of Applied Physics, 2011, 110, .	2.5	14
131	Surface Selectivity of Calcite on Self-Assembled Monolayers. Journal of Physical Chemistry C, 2013, 117, 5154-5163.	3.1	14
132	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
133	The energy of formation of alkali metal ion interstitials in zinc selenide. Journal of Physics C: Solid State Physics, 1981, 14, 5049-5054.	1.5	13
134	The electrical impedance of single-crystal urania at elevated temperatures. Journal of Nuclear Materials, 1988, 154, 245-252.	2.7	13
135	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
136	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
137	The Analysis of Impedance Spectra for Coreâ€“Shell Microstructures: Why a Multiformalism Approach is Essential. Advanced Functional Materials, 2019, 29, 1904036.	14.9	13
138	Interaction of stable aggregates drives the precipitation of calcium phosphate in supersaturated solutions. CrystEngComm, 2019, 21, 6354-6364.	2.6	13
139	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
140	Understanding crystal nucleation mechanisms: where do we stand? General discussion. Faraday Discussions, 0, 235, 219-272.	3.2	13
141	Calculation of local and gap mode frequencies from impurities in alkali halide crystals. Journal of Physics C: Solid State Physics, 1986, 19, 6153-6167.	1.5	12
142	The pressure dependence of the dielectric constant and electrical conductivity of single crystal uranium dioxide. Journal of Nuclear Materials, 1987, 150, 17-23.	2.7	12
143	The Practical Calculation of Interionic Potentials. Molecular Simulation, 1990, 4, 255-268.	2.0	12
144	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

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145	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
146	Study of defect structure of calcium sulphide. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1984, 49, 135-141.	0.6	11
147	A comparison of methods for calculating defect entropies in ionic crystals. Journal of Physics C: Solid State Physics, 1988, 21, 5465-5472.	1.5	11
148	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
149	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
150	Electronic structure of the V-and related centres in alkaline earth oxides. Journal of Physics C: Solid State Physics, 1979, 12, 3931-3940.	1.5	10
151	Calculation of the oxygen potential in the mixed oxide (U, Pu)O2 â^' x. Journal of Nuclear Materials, 1984, 125, 125-137.	2.7	10
152	The dielectric constant of UO2 below the NeÂ´el point. Journal of Nuclear Materials, 1987, 149, 18-20.	2.7	10
153	Calculation of the entropy of defect processes in ionic solids. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 351.	1.1	10
154	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
155	Characterization of aâ€šiN_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
156	Comparison of molecular dynamics and static simulations of an anion vacancy in cobalt oxide. Journal of Physics C: Solid State Physics, 1987, 20, L677-L680.	1.5	9
157	Simulation of oxygen vacancies at the Siâ€“SiO₂ interface. Radiation Effects and Defects in Solids, 1995, 134, 179-183.	1.2	9
158	Simulations of monosaccharide on calcite surfaces. Mineralogical Magazine, 2008, 72, 295-299.	1.4	9
159	Frontispiece: Ion Association in Lanthanide Chloride Solutions. Chemistry - A European Journal, 2019, 25, .	3.3	9
160	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
161	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
162	Cohesion and polymorphism in solid rubidium chloride. Journal of Physics Condensed Matter, 2006, 18, 683-702.	1.8	8

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163	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
164	Defects and clusters in UO2 and (U, Pu)O2. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1177.	1.1	7
165	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
166	Atomistic simulations of surface diffusion and segregation in ceramics. Computational Materials Science, 2006, 36, 54-59.	3.0	7
167	Stoichiometrically graded SiNx for improved surface passivation in high performance solar cells. Journal of Applied Physics, 2012, 112, .	2.5	7
168	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
169	Thin films of wÃ¼rtzite materialsâ€”AlN vs. AlP. Journal of Crystal Growth, 2006, 294, 111-117.	1.5	6
170	Order parameter and connectivity topology analysis of crystalline ceramics for nuclear waste immobilization. Journal of Physics Condensed Matter, 2014, 26, 485011.	1.8	6
171	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
172	Cation diffusion in alkaline-earth oxides. Journal of Physics C: Solid State Physics, 1987, 20, 5281-5292.	1.5	5
173	The V_kcentre in NaCl. Radiation Effects and Defects in Solids, 1991, 119-121, 27-32.	1.2	5
174	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
175	Ion Association in Lanthanide Chloride Solutions. Chemistry - A European Journal, 2019, 25, 8725-8740.	3.3	5
176	Interionic Potentials: A Users Guide. , 1991, , 159-182.		4
177	Simulation Studies of Oxide Materials. Molecular Simulation, 1997, 20, 27-39.	2.0	4
178	Simulating surface diffusion and surface growth in ceramics. Dalton Transactions, 2004, , 3071.	3.3	4
179	Invited review: Mesoscopic modelling: Materials at the appropriate scale. Materials Science and Technology, 2009, 25, 460-465.	1.6	4
180	Ultrathin oxide films and heterojunctions: CaO layers on BaO and SrO. Physical Chemistry Chemical Physics, 2009, 11, 3217.	2.8	4

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