C Richard A Catlow

List of Publications by Year
in descending order

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831 papers	43,701 citations	1980 101 h-index	5101 166 g-index
886 all docs	886 docs citations	886 times ranked	30633 citing authors

#	Article	IF	Citations
1	Band alignment of rutile and anatase TiO2. Nature Materials, 2013, 12, 798-801.	13.3	1,924
2	Potential models for ionic oxides. Journal of Physics C: Solid State Physics, 1985, 18, 1149-1161.	1.5	1,069
3	QUASI: A general purpose implementation of the QM/MM approach and its application to problems in catalysis. Computational and Theoretical Chemistry, 2003, 632, 1-28.	1.5	887
4	Radiation effects in crystalline ceramics for the immobilization of high-level nuclear waste and plutonium. Journal of Materials Research, 1998, 13, 1434-1484.	1.2	842
5	Interatomic potentials for SiO2. Journal of the Chemical Society Chemical Communications, 1984, , 1271.	2.0	486
6	The role of oxygen vacancies on ceria surfaces in the oxidation of carbon monoxide. Surface Science, 1994, 316, 329-336.	0.8	479
7	Advances in theory and their application within the field of zeolite chemistry. Chemical Society Reviews, 2015, 44, 7044-7111.	18.7	405
8	Oxygen Ion Migration in Perovskite-Type Oxides. Journal of Solid State Chemistry, 1995, 118, 125-132.	1.4	404
9	Identification of single-site gold catalysis in acetylene hydrochlorination. Science, 2017, 355, 1399-1403.	6.0	380
10	Bridging hydrodyl groups in zeolitic catalysts: a computer simulation of their structure, vibrational properties and acidity in protonated faujasites (Hî—‚Y zeolites). Chemical Physics Letters, 1992, 188, 320-325.	1.2	370
11	Interionic potentials for alkali halides. Journal of Physics C: Solid State Physics, 1977, 10, 1395-1412.	1.5	346
12	Relative energies of surface and defect states: ab initio calculations for the MgO (001) surface. Surface Science, 2000, 450, 153-170.	0.8	336
13	Computer Simulation Studies of Zeolite Structure. Molecular Simulation, 1988, 1, 207-224.	0.9	326
14	The prediction of inorganic crystal structures using a genetic algorithm and energy minimisation. Physical Chemistry Chemical Physics, 1999, 1, 2535-2542.	1.3	322
15	Defect energetics inÎ±-Al2O3and rutile TiO2. Physical Review B, 1982, 25, 1006-1026.	1.1	313
16	Strain and Orientation Modulated Bandgaps and Effective Masses of Phosphorene Nanoribbons. Nano Letters, 2014, 14, 4607-4614.	4.5	306
17	De novo design of structure-directing agents for the synthesis of microporous solids. Nature, 1996, 382, 604-606.	13.7	302
18	Defect studies of doped and undoped barium titanate using computer simulation techniques. Journal of Physics and Chemistry of Solids, 1986, 47, 89-97.	1.9	300

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19	Local geometry ofFe3+ions on the potassium sites inKTaO3. Physical Review B, 1993, 47, 14-19.	1.1	293
20	EXAFS Study of Yttria-Stabilized Zirconia. Journal of the American Ceramic Society, 1986, 69, 272-277.	1.9	286
21	Designer Titania-Supported Auâ€“Pd Nanoparticles for Efficient Photocatalytic Hydrogen Production. ACS Nano, 2014, 8, 3490-3497.	7.3	279
22	Dopant ion radius and ionic conductivity in cerium dioxide. Solid State Ionics, 1983, 8, 109-113.	1.3	274
23	Self-consistent interatomic potentials for the simulation of binary and ternary oxides. Journal of Materials Chemistry, 1994, 4, 831.	6.7	273
24	Defects and diffusion in pyrochlore structured oxides. Solid State Ionics, 1998, 112, 173-183.	1.3	261
25	Controlling Bulk Conductivity in Topological Insulators: Key Role of Antiâ€Site Defects. Advanced Materials, 2012, 24, 2154-2158.	11.1	258
26	Defect aggregation in anion-excess fluorites. Dopant monomers and dimers. Physical Review B, 1982, 25, 6425-6438.	1.1	238
27	Computer Simulation Studies of Strontium Titanate. Journal of the American Ceramic Society, 1995, 78, 421-428.	1.9	232
28	Computer-simulation studies of intrinsic defects inLiNbO3crystals. Physical Review B, 1989, 40, 11909-11916.	1.1	216
29	Structure and Stability of Small TiO2Nanoparticles. Journal of Physical Chemistry B, 2005, 109, 15741-15748.	1.2	212
30	Ionicity in solids. Journal of Physics C: Solid State Physics, 1983, 16, 4321-4338.	1.5	209
31	Recent developments and perspectives in CdS-based photocatalysts for water splitting. Journal of Materials Chemistry A, 2020, 8, 20752-20780.	5.2	203
32	Theoretical study of the stabilization of cubic-phaseZrO2by impurities. Physical Review B, 1994, 49, 11560-11571.	1.1	202
33	PTCR Effect in BaTiO3. Journal of the American Ceramic Society, 1985, 68, 555-558.	1.9	195
34	A Multilateral Mechanistic Study into Asymmetric Transfer Hydrogenation in Water. Chemistry - A European Journal, 2008, 14, 7699-7715.	1.7	194
35	Predicting the Templating Ability of Organic Additives for the Synthesis of Microporous Materials. The Journal of Physical Chemistry, 1995, 99, 11194-11202.	2.9	190
36	Structure and stability of the (001) Î±-quartz surface. Physical Chemistry Chemical Physics, 2007, 9, 2146-2152.	1.3	189

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37	Bio-inspired CO₂conversion by iron sulfide catalysts under sustainable conditions. Chemical Communications, 2015, 51, 7501-7504.	2.2	188
38	Symmetry-adapted configurational modelling of fractional site occupancy in solids. Journal of Physics Condensed Matter, 2007, 19, 256201.	0.7	182
39	Modeling of Silicon Substitution in SAPO-5 and SAPO-34 Molecular Sieves. Journal of Physical Chemistry B, 1997, 101, 5249-5262.	1.2	179
40	Structure, stability and work functions of the low index surfaces of pure indium oxide and Sn-doped indium oxide (ITO) from density functional theory. Journal of Materials Chemistry, 2010, 20, 10438.	6.7	177
41	Modelling nano-clusters and nucleation. Physical Chemistry Chemical Physics, 2010, 12, 786-811.	1.3	174
42	Shell model calculations of the energies of formation of point defects in alkaline earth fluorides. Journal of Physics C: Solid State Physics, 1973, 6, 1325-1339.	1.5	171
43	A New High-Flux Chemical and Materials Crystallography Station at the SRS Daresbury. 1. Design, Construction and Test Results. Journal of Synchrotron Radiation, 1997, 4, 279-286.	1.0	171
44	Calculations of defect clustering in Fe1-xO. Journal of Physics C: Solid State Physics, 1975, 8, 3267-3279.	1.5	170
45	X-ray Absorption Spectroscopic Study of BrÃ¸nsted, Lewis, and Redox Centers in Cobalt-Substituted Aluminum Phosphate Catalysts. The Journal of Physical Chemistry, 1996, 100, 8977-8985.	2.9	159
46	Molecular dynamics studies of hydrocarbon diffusion in zeolites. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1947.	1.7	156
47	The relaxation of molecular crystal structures using a distributed multipole electrostatic model. Journal of Computational Chemistry, 1995, 16, 628-647.	1.5	154
48	Study of Surface Segregation of Antimony on SnO2 Surfaces by Computer Simulation Techniques. Journal of Physical Chemistry B, 1999, 103, 10644-10650.	1.2	154
49	Point defects in ZnO. Faraday Discussions, 2007, 134, 267-282.	1.6	151
50	SAPO-18 Catalysts and Their Broensted Acid Sites. The Journal of Physical Chemistry, 1994, 98, 10216-10224.	2.9	149
51	Arsenic incorporation into FeS2 pyrite and its influence on dissolution: A DFT study. Geochimica Et Cosmochimica Acta, 2007, 71, 624-630.	1.6	149
52	Anharmonicity in the High-Temperature<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>C</mml:mi><mml:mi>m</mml:mi><mml:mi>c</mml:mi><mml:mi>m</mml:mi></mml:math>Phase of SnSe: Soft Modes and Three-Phonon Interactions. Physical Review Letters, 2016, 117, 075502.	8.1	147
53	Evolutionary programming techniques for predicting inorganic crystal structures. Journal of Materials Chemistry, 1995, 5, 1269.	6.7	146
54	Computer modelling of solid-state inorganic materials. Nature, 1990, 347, 243-248.	13.7	145

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55	Comparison of the Bulk and Surface Properties of Ceria and Zirconia by ab Initio Investigations. Journal of Physical Chemistry B, 1999, 103, 10158-10170.	1.2	145
56	Quantum Chemical Study of the Mechanism of Partial Oxidation Reactivity in Titanosilicate Catalysts:â€‰ Active Site Formation, Oxygen Transfer, and Catalyst Deactivation. Journal of Physical Chemistry B, 1999, 103, 1084-1095.	1.2	142
57	Computing the location and energetics of organic molecules in microporous adsorbents and catalysts: a hybrid approach applied to isometric butenes in a model zeolite. Chemical Physics Letters, 1991, 186, 137-142.	1.2	141
58	Why Are Polar Surfaces of ZnO Stable?. Chemistry of Materials, 2017, 29, 5306-5320.	3.2	141
59	The structural properties of the oxygen conducting Î´ phase of Bi2O3. Journal of Physics C: Solid State Physics, 1983, 16, L561-L566.	1.5	139
60	A structural basis for ionic diffusion in oxide glasses. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1991, 64, 1059-1072.	0.8	137
61	The calculation of defect parameters in UO₂. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1986, 53, 27-50.	0.8	135
62	Nitrogen Activation in a Marsâ€“van Krevelen Mechanism for Ammonia Synthesis on Co₃Mo₃N. Journal of Physical Chemistry C, 2015, 119, 28368-28376.	1.5	135
63	Oxidation states and ionicity. Nature Materials, 2018, 17, 958-964.	13.3	135
64	Defect aggregation in anion-excess fluorites II. Clusters containing more than two impurity atoms. Journal of Solid State Chemistry, 1984, 51, 159-169.	1.4	134
65	Shell and breathing shell model calculations for defect formation energies and volumes in magnesium oxide. Journal of Physics C: Solid State Physics, 1976, 9, 419-430.	1.5	133
66	Brillouin scattering and theoretical studies of high-temperature disorder in fluorite crystals. Journal of Physics C: Solid State Physics, 1978, 11, 3197-3212.	1.5	132
67	Direct observations of the dopant environment in fluorites using EXAFS. Nature, 1984, 312, 601-604.	13.7	132
68	Siting of Al and bridging hydroxyl groups in ZSM-5: A computer simulation study. Zeolites, 1992, 12, 20-23.	0.9	132
69	The architecture of catalytically active centers in titanosilicate (TS-1) and related selective-oxidation catalysts. Physical Chemistry Chemical Physics, 2000, 2, 4812-4817.	1.3	130
70	Bandgap Engineering of Organic Semiconductors for Highly Efficient Photocatalytic Water Splitting. Advanced Energy Materials, 2018, 8, 1801084.	10.2	127
71	Ion transport and interatomic potentials in the alkaline-earth-fluoride crystals. Journal of Physics C: Solid State Physics, 1977, 10, 1627-1640.	1.5	125
72	Computational and EXAFS Study of the Nature of the Ti(IV) Active Sites in Mesoporous Titanosilicate Catalysts. Journal of Physical Chemistry B, 1997, 101, 4232-4237.	1.2	125

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73	Lithium Intercalation into Vanadium Pentoxide:Â a Theoretical Study. Chemistry of Materials, 1999, 11, 1990-1998.	3.2	122
74	Quantum-chemical studies of alkene chemisorption in chabazite: A comparison of cluster and embedded-cluster models. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 3401-3408.	1.7	121
75	An in Situ Energy-Dispersive X-ray Diffraction Study of the Hydrothermal Crystallization of Zeolite A. 1. Influence of Reaction Conditions and Transformation into Sodalite. Journal of Physical Chemistry B, 2001, 105, 83-90.	1.2	121
76	Anab InitioHartreeâ^'Fock Study of the Cubic and Tetragonal Phases of Bulk Tungsten Trioxide. Journal of the American Chemical Society, 1996, 118, 12174-12182.	6.6	120
77	Advances in computational studies of energy materials. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 3379-3456.	1.6	119
78	Surface Structures and Crystal Morphology of ZnS:â€‰ Computational Study. Journal of Physical Chemistry B, 2002, 106, 11002-11008.	1.2	116
79	Structure and Stability of Silica Species in SAPO Molecular Sieves. The Journal of Physical Chemistry, 1996, 100, 6722-6730.	2.9	115
80	Oxygen Diffusion in LaMnO3and LaCoO3Perovskite-Type Oxides: A Molecular Dynamics Study. Journal of Solid State Chemistry, 1996, 124, 230-237.	1.4	114
81	Computer-simulation studies of extrinsic defects inLiNbO3crystals. Physical Review B, 1991, 44, 4877-4883.	1.1	113
82	Polymorph Engineering of TiO₂: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. Chemistry of Materials, 2015, 27, 3844-3851.	3.2	113
83	Tandem Site- and Size-Controlled Pd Nanoparticles for the Directed Hydrogenation of Furfural. ACS Catalysis, 2017, 7, 2266-2274.	5.5	113
84	Computer modelling of barium titanate. Radiation Effects, 1983, 73, 307-314.	0.4	112
85	Irradiationâ€induced defects in alkali halide crystals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1980, 42, 123-150.	0.8	111
86	Ab Initio Studies of Silica-Based Clusters. Part I. Energies and Conformations of Simple Clusters. Journal of Physical Chemistry A, 1999, 103, 3252-3267.	1.1	111
87	Modelling the effect of water on the surface structure and stability of forsterite. Physics and Chemistry of Minerals, 2000, 27, 332-341.	0.3	110
88	Computer Modeling of Nucleation, Growth, and Templating in Hydrothermal Synthesis. Chemistry of Materials, 1998, 10, 3249-3265.	3.2	109
89	Defect structures and migration mechanisms in oxide pyrochlores. Solid State Ionics, 1985, 17, 159-167.	1.3	108
90	Defects in LiNbO3â€”II. Computer simulation. Journal of Physics and Chemistry of Solids, 1991, 52, 201-210.	1.9	108

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91	Calculated bulk and surface properties of sulfates. Faraday Discussions, 1993, 95, 273.	1.6	108
92	Simulation studies of the structure and energetics of sorbed molecules in high-silica zeolites. 1. Hydrocarbons. The Journal of Physical Chemistry, 1991, 95, 4038-4044.	2.9	107
93	Surface oxygen vacancy formation on CeO2 and its role in the oxidation of carbon monoxide. Journal of the Chemical Society Chemical Communications, 1992, , 977.	2.0	107
94	Transition Metal Oxide Chemistry:â€‰ Electronic Structure Study of WO3, ReO3, and NaWO3. Journal of Physical Chemistry B, 1997, 101, 3945-3952.	1.2	107
95	Kinetic Insights into the Role of the Solvent in the Polymorphism of 5-Fluorouracil from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2006, 110, 3323-3329.	1.2	107
96	Periodic ab initio determination of interatomic potentials for alumina. Modelling and Simulation in Materials Science and Engineering, 1992, 1, 73-81.	0.8	106
97	Oligomerization and Cyclization Processes in the Nucleation of Microporous Silicas. Angewandte Chemie - International Edition, 2005, 44, 3082-3086.	7.2	106
98	Structures of Zinc Oxide Nanoclusters: As Found by Revolutionary Algorithm Techniques. Journal of Physical Chemistry C, 2008, 112, 18860-18875.	1.5	106
99	Zinc oxide: A case study in contemporary computational solid state chemistry. Journal of Computational Chemistry, 2008, 29, 2234-2249.	1.5	105
100	A study of cation environment and movement during dehydration and reduction of nickel-exchanged zeolite Y by x-ray absorption and diffraction. The Journal of Physical Chemistry, 1991, 95, 4514-4521.	2.9	104
101	From CO2 to Methanol by Hybrid QM/MM Embedding This work was supported by EU Esprit IV project 25047. S.A.F. is grateful to ICI and Synetix for funding. K. Waugh, L. Whitmore, S. Cristol, and P. Sushko are thanked for their helpful insights. QM/MM=quantum mechanics/molecular mechanics.. Angewandte Chemie - International Edition, 2001, 40, 4437.	7.2	102
102	Structure and Properties of ZnS Nanoclusters. Journal of Physical Chemistry B, 2005, 109, 2703-2709.	1.2	102
103	An ab initio study of methanol adsorption in zeolites. Chemical Physics Letters, 1993, 216, 155-161.	1.2	101
104	Structural and dynamical studies of Î´-Bi2O3 oxide ion conductors. Journal of Solid State Chemistry, 1986, 63, 8-15.	1.4	99
105	Computational Studies of Protons in Perovskite-Structured Oxides. The Journal of Physical Chemistry, 1995, 99, 14614-14618.	2.9	98
106	Designing a Solid Catalyst for the Selective Low-Temperature Oxidation of Cyclohexane to Cyclohexanone. Angewandte Chemie International Edition in English, 1997, 36, 1639-1642.	4.4	98
107	Ab Initio Studies of Silica-Based Clusters. Part II. Structures and Energies of Complex Clusters. Journal of Physical Chemistry A, 1999, 103, 3268-3284.	1.1	97
108	Hybrid QM/MM embedding approach for the treatment of localized surface states in ionic materials. International Journal of Quantum Chemistry, 2004, 99, 695-712.	1.0	97

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109	The basic atomic processes of corrosion I. Electronic conduction in MnO, CoO and NiO. Philosophical Magazine and Journal, 1977, 35, 177-187.	1.8	96
110	Pseudopotential periodic hartree-fock study of rutile TiO2. Journal of Physics and Chemistry of Solids, 1991, 52, 1005-1009.	1.9	96
111	Anab initio Hartreeâ€“Fock study of Î±-MoO3. Journal of Materials Chemistry, 1997, 7, 959-967.	6.7	96
112	Surface Energies Control the Self-Organization of Oriented In₂O₃ Nanostructures on Cubic Zirconia. Nano Letters, 2010, 10, 3740-3746.	4.5	96
113	An ab-initio Hartree-Fock study of ?-quartz and stishovite. Physics and Chemistry of Minerals, 1990, 17, 353.	0.3	95
114	Defects and Oxide Ion Migration in the Solid Oxide Fuel Cell Cathode Material LaFeO₃. Chemistry of Materials, 2016, 28, 8210-8220.	3.2	95
115	Electrochemical upgrading of biomass-derived 5-hydroxymethylfurfural and furfural over oxygen vacancy-rich NiCoMn-layered double hydroxides nanosheets. Green Chemistry, 2021, 23, 4034-4043.	4.6	95
116	Au-ZSM-5 catalyses the selective oxidation of CH4 to CH3OH and CH3COOH using O2. Nature Catalysis, 2022, 5, 45-54.	16.1	95
117	Computational approaches to the determination of active site structures and reaction mechanisms in heterogeneous catalysts. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2005, 363, 913-936.	1.6	94
118	Computer modelling studies of defects and valence states in La2CuO4. Journal of Physics C: Solid State Physics, 1988, 21, L109-L117.	1.5	91
119	Water-like melting behaviour of SiO₂ investigated by the molecular dynamics simulation technique. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1989, 60, 753-775.	0.6	89
120	An ab-initio Hartree-Fock perturbed-cluster study of neutral defects in LiF. Modelling and Simulation in Materials Science and Engineering, 1993, 1, 165-187.	0.8	88
121	Diffusion of Benzene and Propylene in MCM-22 Zeolite. A Molecular Dynamics Study. Journal of Physical Chemistry B, 1999, 103, 5187-5196.	1.2	88
122	Computer Simulation Studies of Transport in Solids. Annual Review of Materials Research, 1986, 16, 517-548.	5.5	87
123	Identification and Characterization of Active Sites and Their Catalytic Processesâ€”the Cu/ZnO Methanol Catalyst. Topics in Catalysis, 2003, 24, 161-172.	1.3	87
124	Low-T Mechanisms of Ammonia Synthesis on Co₃Mo₃N. Journal of Physical Chemistry C, 2018, 122, 6078-6082.	1.5	87
125	Inorganic crystal structure prediction using simplified potentials and experimental unit cells: application to the polymorphs of titanium dioxide. Journal of Materials Chemistry, 1993, 3, 531.	6.7	86
126	Active Nature of Primary Amines during Thermal Decomposition of Nickel Dithiocarbamates to Nickel Sulfide Nanoparticles. Chemistry of Materials, 2014, 26, 6281-6292.	3.2	86

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127	Synthesis of a Small-Pore Microporous Material Using a Computationally Designed Template. Angewandte Chemie International Edition in English, 1997, 36, 2675-2677.	4.4	85
128	Computer modelling as a technique in materials chemistry. Journal of Materials Chemistry, 1994, 4, 781.	6.7	84
129	The Three-Dimensional Structure of the Titanium-Centered Active Site during Steady-State Catalytic Epoxidation of Alkenes. Journal of Physical Chemistry B, 2001, 105, 9028-9030.	1.2	84
130	Fine Structures of Zeolite-Linde-L (LTL): Surface Structures, Growth Unit and Defects. Chemistry - A European Journal, 2004, 10, 5031-5040.	1.7	84
131	Synergistic ultraviolet and visible light photo-activation enables intensified low-temperature methanol synthesis over copper/zinc oxide/alumina. Nature Communications, 2020, 11, 1615.	5.8	84
132	Structural properties of titanium sites in Ti-ZSM5. Catalysis Letters, 1993, 22, 251-257.	1.4	83
133	Transport in doped fluorite oxides. Solid State Ionics, 1984, 12, 67-73.	1.3	82
134	Atomistic mechanisms of ionic transport in fast-ion conductors. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 1167.	1.7	82
135	Computational Evidence of Bubble ZnS Clusters. Journal of Physical Chemistry B, 2003, 107, 10337-10340.	1.2	82
136	Bulk and surface properties of metal carbides: implications for catalysis. Physical Chemistry Chemical Physics, 2018, 20, 6905-6916.	1.3	82
137	The contribution of vacancy defects to mass transport in alkali halides-an assessment using theoretical calculations of defect energies. Journal of Physics C: Solid State Physics, 1979, 12, 451-464.	1.5	81
138	Theoretical studies of protons in sodium hydroxide. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1985, 51, 107-117.	0.6	81
139	Molecular dynamics study of the effect of doping and disorder on diffusion in gadolinium zirconate. Solid State Ionics, 1998, 112, 185-195.	1.3	80
140	Experimental and computational study of the gas-sensor behaviour and surface chemistry of the solid-solution Cr2â€“xTixO3 (x â‰¤ 0.5). Journal of Materials Chemistry, 2002, 12, 667-675.	6.7	80
141	On the cation distribution of spinels. Journal of Physics and Chemistry of Solids, 1988, 49, 53-57.	1.9	79
142	Structure of Iron-Substituted ZSM-5. The Journal of Physical Chemistry, 1995, 99, 2377-2383.	2.9	79
143	Clustering of Glycine Molecules in Aqueous Solution Studied by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 7280-7288.	1.2	79
144	Automated procedure to determine the thermodynamic stability of a material and the range of chemical potentials necessary for its formation relative to competing phases and compounds. Computer Physics Communications, 2014, 185, 330-338.	3.0	79

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145	The basic atomic processes of corrosion II. Defect structures and cation transport in transition-metal oxides. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1979, 40, 161-172.	0.8	78
146	The defect structure of anion deficient ZrO 2. Solid State Ionics, 1981, 5, 539-542.	1.3	78
147	An embedded cluster study of the formation of water on interstellar dust grains. Physical Chemistry Chemical Physics, 2009, 11, 5431.	1.3	78
148	Structure prediction of transition-metal oxides using energy-minimization techniques. Acta Crystallographica Section B: Structural Science, 1984, 40, 195-200.	1.8	77
149	Interatomic potentials for oxides. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1988, 58, 123-141.	0.8	77
150	Interactions at the Organic/Inorganic Interface:Â Molecular Modeling of the Interaction between Diphosphonates and the Surfaces of Barite Crystals. Journal of the American Chemical Society, 1996, 118, 642-648.	6.6	77
151	Combining Xâ€ray absorption with Xâ€ray diffraction for the structural elucidation of catalysts. Topics in Catalysis, 2000, 10, 255-264.	1.3	75
152	Unique Organicâ"Inorganic Interactions Leading to a Structure-Directed Microporous Aluminophosphate Crystallization as Observed with in situ Raman Spectroscopy. Journal of the American Chemical Society, 2006, 128, 11744-11745.	6.6	75
153	Defect clusters in doped fluorite crystals. Journal of Physics C: Solid State Physics, 1973, 6, L64-L70.	1.5	74
154	The defect properties of anion-excess alkaline-earth fluorides. I. Low defect concentrations. Journal of Physics C: Solid State Physics, 1976, 9, 1845-1857.	1.5	74
155	The thermodynamics of characteristic defect parameters. Journal of Physics C: Solid State Physics, 1981, 14, L121-L125.	1.5	74
156	Oxygen diffusion in UO2, ThO2 and PuO2. A review. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1157.	1.1	74
157	Atomistic Simulation of Defect Structures and Ion Transport in alpha-Fe2O3 and alpha-Cr2O3. Journal of the American Ceramic Society, 1988, 71, 42-49.	1.9	74
158	On the structure and coordination of the oxygen-donating species in Tiâ†'MCM-41/TBHP oxidation catalysts: a density functional theory and EXAFS study. Physical Chemistry Chemical Physics, 2002, 4, 1228-1240.	1.3	74
159	Hole localization in [AlO4]0 defects in silica materials. Journal of Chemical Physics, 2005, 122, 144704.	1.2	74
160	Structural selectivity of supported Pd nanoparticles for catalytic NH3 oxidation resolved using combined operando spectroscopy. Nature Catalysis, 2019, 2, 157-163.	16.1	74
161	Defect Equilibria in Transition Metal Oxides. Journal of the American Ceramic Society, 1981, 64, 234-236.	1.9	73
162	Deep vs shallow nature of oxygen vacancies and consequent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math>-type carrier concentrations in transparent conducting oxides. Physical Review Materials, 2018, 2, .	0.9	73

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163	A computer modeling study of defect and dopant states in SnO2. Journal of Solid State Chemistry, 1990, 85, 65-75.	1.4	72
164	Computer simulation of the structure of silica glass. Journal of Non-Crystalline Solids, 1993, 159, 184-186.	1.5	72
165	Influence of Organic Templates on the Structure and on the Concentration of Framework Metal Ions in Microporous Aluminophosphate Catalysts. Chemistry of Materials, 1996, 8, 1112-1118.	3.2	72
166	Computer modelling of the defect structure of non-stoichiometric binary transition metal oxides. Journal of Physics and Chemistry of Solids, 1990, 51, 477-506.	1.9	71
167	The potential of manganese nitride based materials as nitrogen transfer reagents for nitrogen chemical looping. Applied Catalysis B: Environmental, 2018, 223, 60-66.	10.8	71
168	Trapping and solution of fission Xe in UO2.. Journal of Nuclear Materials, 1985, 127, 161-166.	1.3	70
169	Modeling Aqueous Silica Chemistry in Alkali Media. Journal of Physical Chemistry C, 2007, 111, 18155-18158.	1.5	70
170	Determination of the Nitrogen Vacancy as a Shallow Compensating Center in GaN Doped with Divalent Metals. Physical Review Letters, 2015, 114, 016405.	2.9	70
171	Generating MnO2Nanoparticles Using Simulated Amorphization and Recrystallization. Journal of the American Chemical Society, 2005, 127, 12828-12837.	6.6	69
172	Properties of small TiO2, ZrO2and HfO2nanoparticles. Journal of Materials Chemistry, 2006, 16, 1927-1933.	6.7	69
173	Surface Segregation of Metal Ions in Cerium Dioxide. The Journal of Physical Chemistry, 1994, 98, 13625-13630.	2.9	68
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