Stephen C Parker

List of Publications by Year
in descending order

272	14,399	14644 66	24961 109
papers	citations	h-index	g-index

284	284	284	13330
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The electronic structure of oxygen vacancy defects at the low index surfaces of ceria. Surface Science, 2005, 595, 223-232.	0.8	690
2	Density functional theory studies of the structure and electronic structure of pure and defective low index surfaces of ceria. Surface Science, 2005, 576, 217-229.	0.8	683
3	Surface Structure and Morphology of Calcium Carbonate Polymorphs Calcite, Aragonite, and Vaterite:Â An Atomistic Approach. Journal of Physical Chemistry B, 1998, 102, 2914-2922.	1.2	492
4	Atomistic simulation of dislocations, surfaces and interfaces in MgO. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 433.	1.7	453
5	ElAM: A computer program for the analysis and representation of anisotropic elastic properties. Computer Physics Communications, 2010, 181, 2102-2115.	3.0	321
6	Atomistic simulation of the surface structure of the TiO2 polymorphs rutileand anatase. Journal of Materials Chemistry, 1997, 7, 563-568.	6.7	294
7	Free Energy of Adsorption of Water and Metal Ions on the {101Ì„4} Calcite Surface. Journal of the American Chemical Society, 2004, 126, 10152-10161.	6.6	276
8	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. Physical Review B, 2014, 89, .	1.1	212
9	Modeling the Surface Structure and Stability of Î±-Quartz. Journal of Physical Chemistry B, 1999, 103, 1270-1277.	1.2	211
10	Water Adsorption and Its Effect on the Stability of Low Index Stoichiometric and Reduced Surfaces of Ceria. Journal of Physical Chemistry C, 2012, 116, 7073-7082.	1.5	204
11	Atomistic simulation of the effect of molecular adsorption of water on the surface structure and energies of calcite surfaces. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 467-475.	1.7	193
12	Molecular-dynamics simulation of MgO surfaces in liquid water using a shell-model potential for water. Physical Review B, 1998, 58, 13901-13908.	1.1	189
13	Lattice dynamics of the tin sulphides SnS₂, SnS and Sn₂S₃: vibrational spectra and thermal transport. Physical Chemistry Chemical Physics, 2017, 19, 12452-12465.	1.3	187
14	Rutile (Î²-)MnO₂ Surfaces and Vacancy Formation for High Electrochemical and Catalytic Performance. Journal of the American Chemical Society, 2014, 136, 1418-1426.	6.6	186
15	: A force field database for cementitious materials including validations, applications and opportunities. Cement and Concrete Research, 2017, 102, 68-89.	4.6	186
16	Lithium Insertion and Transport in the TiO₂â^'B Anode Material: A Computational Study. Chemistry of Materials, 2009, 21, 4778-4783.	3.2	169
17	Modelling of the thermal dependence of structural and elastic properties of calcite, CaCO3. Physics and Chemistry of Minerals, 1996, 23, 89.	0.3	166
18	Ab initiocalculation of the origin of the distortion of Î±-PbO. Physical Review B, 1999, 59, 8481-8486.	1.1	160

#	Article	IF	Citations
19	Oxidising CO to CO2 using ceria nanoparticles. Physical Chemistry Chemical Physics, 2005, 7, 2936.	1.3	159
20	Origin of the Lone Pair of Î±-PbO from Density Functional Theory Calculations. Journal of Physical Chemistry B, 1999, 103, 1258-1262.	1.2	157
21	Atomistic Simulation of the Effect of Dissociative Adsorption of Water on the Surface Structure and Stability of Calcium and Magnesium Oxide. The Journal of Physical Chemistry, 1995, 99, 17219-17225.	2.9	152
22	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.	2.9	147
23	Atomistic Simulation of the Dissociative Adsorption of Water on Calcite Surfaces. Journal of Physical Chemistry B, 2003, 107, 7676-7682.	1.2	141
24	Phase stability and transformations in the halide perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CsSnI</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review B, 2015, 91, .	1.1	138
25	The lattice dynamics and thermodynamics of the Mg2SiO4 polymorphs. Physics and Chemistry of Minerals, 1987, 15, 181-190.	0.3	125
26	The MD simulation of the equation of state of MgO: Application as a pressure calibration standard at high temperature and high pressure. American Mineralogist, 2000, 85, 312-316.	0.9	124
27	Surface properties of Î±-MnO₂: relevance to catalytic and supercapacitor behaviour. Journal of Materials Chemistry A, 2014, 2, 15509-15518.	5.2	121
28	Ab initiomorphology and surface thermodynamics ofÎ±â^'Al2O3. Physical Review B, 2004, 69, .	1.1	117
29	Reduction of NO2on Ceria Surfaces. Journal of Physical Chemistry B, 2006, 110, 2256-2262.	1.2	117
30	Computer simulations of the structural and physical properties of the olivine and spinel polymorphs of Mg2SiO4. Physics and Chemistry of Minerals, 1984, 10, 209-216.	0.3	114
31	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
32	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
33	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
34	CeO2catalysed conversion of CO, NO2and NO from first principles energetics. Physical Chemistry Chemical Physics, 2006, 8, 216-218.	1.3	107
35	The Atomic-Level Structure of Cementitious Calcium Aluminate Silicate Hydrate. Journal of the American Chemical Society, 2020, 142, 11060-11071.	6.6	107
36	Lithium Coordination Sites in Li_xTiO₂(B): A Structural and Computational Study. Chemistry of Materials, 2010, 22, 6426-6432.	3.2	104

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37	Atomistic Simulation of the Surface Energy of Spinel MgAl₂O₄. Journal of the American Ceramic Society, 2000, 83, 2082-2084.	1.9	101
38	Strain and Architecture-Tuned Reactivity in Ceria Nanostructures; Enhanced Catalytic Oxidation of CO to CO₂. Chemistry of Materials, 2012, 24, 1811-1821.	3.2	100
39	Nanostructuring of Î²-MnO₂: The Important Role of Surface to Bulk Ion Migration. Chemistry of Materials, 2013, 25, 536-541.	3.2	99
40	Structural, electronic and thermoelectric behaviour of CaMnO₃ and CaMnO_(3â^'Î). Journal of Materials Chemistry A, 2014, 2, 14109-14117.	5.2	98
41	Molecular dynamics simulations of the interactions between water and inorganic solids. Journal of Materials Chemistry, 2005, 15, 1454.	6.7	95
42	Tin Monoxide: Structural Prediction from First Principles Calculations with van der Waals Corrections. Journal of Physical Chemistry C, 2011, 115, 19916-19924.	1.5	95
43	Thermal Expansion Behavior of Zeolites and AlPO4s. The Journal of Physical Chemistry, 1995, 99, 10609-10615.	2.9	94
44	Molecular dynamics simulation of crystal dissolution from calcite steps. Physical Review B, 1999, 60, 13792-13799.	1.1	93
45	Modeling the Competitive Adsorption of Water and Methanoic Acid on Calcite and Fluorite Surfaces. Langmuir, 1998, 14, 5900-5906.	1.6	91
46	Structural characterization of amorphous alumina and its polymorphs from first-principles XPS and NMR calculations. Physical Review B, 2011, 83, .	1.1	90
47	Molecular-dynamics simulations of nickel oxide surfaces. Physical Review B, 1995, 52, 5323-5329.	1.1	86
48	Modelling the effect of water on cation exchange in zeolite A. Journal of Materials Chemistry, 2002, 12, 124-131.	6.7	84
49	Shape of CeO2 nanoparticles using simulated amorphisation and recrystallisation. Chemical Communications, 2004, , 2438.	2.2	84
50	The lattice dynamics of forsterite. Mineralogical Magazine, 1987, 51, 157-170.	0.6	83
51	A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor. Nature Communications, 2017, 8, 1800.	5.8	83
52	Atomistic simulation of the surface structure of spinel. Journal of Materials Chemistry, 1994, 4, 813.	6.7	81
53	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. Journal of Chemical Physics, 2015, 143, 064710.	1.2	80
54	Particle Morphology and Lithium Segregation to Surfaces of the Li₇La₃Zr₂O₁₂ Solid Electrolyte. Chemistry of Materials, 2018, 30, 3019-3027.	3.2	80

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55	Surfaceâ€“water interactions in the dolomite problem. Physical Chemistry Chemical Physics, 2001, 3, 3217-3221.	1.3	79
56	An atomistic building block description of C-S-H - Towards a realistic C-S-H model. Cement and Concrete Research, 2018, 107, 221-235.	4.6	78
57	Computer simulation of the structure and stability of forsterite surfaces. Physics and Chemistry of Minerals, 1997, 25, 70-78.	0.3	74
58	Atomistic simulation of hydroxide ions in inorganic solids. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1996, 73, 49-58.	0.6	72
59	Modeling the Surface Structure and Reactivity of Pyrite:Â Introducing a Potential Model for FeS2. Journal of Physical Chemistry B, 2000, 104, 7969-7976.	1.2	72
60	Surface Structure of (101Ì„0) and (112Ì„0) Surfaces of ZnO with Density Functional Theory and Atomistic Simulation. Journal of Physical Chemistry B, 2006, 110, 7985-7991.	1.2	71
61	Environment-mediated structure, surface redox activity and reactivity of ceria nanoparticles. Nanoscale, 2013, 5, 6063.	2.8	71
62	Computer simulation of the crystal morphology of NiO. Modelling and Simulation in Materials Science and Engineering, 1993, 1, 755-760.	0.8	70
63	Simulation of the structure and stability of sphalerite (ZnS) surfaces. American Mineralogist, 1998, 83, 141-146.	0.9	69
64	Surface Segregation of Metal Ions in Cerium Dioxide. The Journal of Physical Chemistry, 1994, 98, 13625-13630.	2.9	68
65	Simulating silicate structures and the structural chemistry of pyroxenoids. Nature, 1982, 295, 658-662.	13.7	67
66	Free energy of adsorption of water and calcium on the {10 1? 4} calcite surfaceElectronic supplementary information (ESI) available: free energy calculations. See http://www.rsc.org/suppdata/cc/b3/b311928a/. Chemical Communications, 2004, , 52.	2.2	67
67	DL_MONTE: a general purpose program for parallel Monte Carlo simulation. Molecular Simulation, 2013, 39, 1240-1252.	0.9	66
68	Computer simulation of the surface structures of WO3. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2049.	1.7	65
69	Effect of Chemisorption and Physisorption of Water on the Surface Structure and Stability of alphaâ€Alumina. Journal of the American Ceramic Society, 1999, 82, 3209-2316.	1.9	63
70	Growth modification of seeded calcite using carboxylic acids: Atomistic simulations. Journal of Colloid and Interface Science, 2010, 346, 226-231.	5.0	63
71	Atomistic simulation of oxide surfaces and their reactivity with water. Faraday Discussions, 1999, 114, 381-393.	1.6	62
72	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.	0.7	61

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73	Particle shapes and surface structures of olivine NaFePO₄ in comparison to LiFePO₄. Physical Chemistry Chemical Physics, 2014, 16, 21788-21794.	1.3	61
74	Computer modelling of inorganic solids and surfaces. Faraday Discussions, 1993, 95, 75.	1.6	60
75	Molecular dynamics simulations of the interaction between the surfaces of polar solids and aqueous solutions. Journal of Materials Chemistry, 2006, 16, 1997.	6.7	60
76	Atomistic simulation of the free energies of dissolution of ions from flat and stepped calcite surfaces. Journal of Crystal Growth, 2006, 294, 103-110.	0.7	60
77	Atomistic simulation of adsorption of water on three-, four- and five-coordinated surface sites of magnesium oxide. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2081.	1.7	58
78	Experimental verification of a predicted negative thermal expansivity of crystalline zeolites. Journal of Physics Condensed Matter, 1993, 5, L329-L332.	0.7	57
79	Electronic structure of the antiferromagneticB1-structured FeO. Physical Review B, 2004, 70, .	1.1	57
80	Modeling absorption and segregation of magnesium and cadmium ions to calcite surfaces: Introducing MgCO3 and CdCO3 potential models. Journal of Chemical Physics, 2000, 112, 4326-4333.	1.2	55
81	Molecular Dynamics Simulations of Electrolyte Solutions at the (100) Goethite Surface. Journal of Physical Chemistry B, 2006, 110, 20491-20501.	1.2	54
82	Cationic Surface Reconstructions on Cerium Oxide Nanocrystals: An Aberration-Corrected HRTEM Study. ACS Nano, 2012, 6, 421-430.	7.3	53
83	Structure prediction of silicate minerals using energy-minimization techniques. Acta Crystallographica Section B: Structural Science, 1984, 40, 200-208.	1.8	49
84	Toward Modeling Clay Mineral Nanoparticles: The Edge Surfaces of Pyrophyllite and Their Interaction with Water. Journal of Physical Chemistry C, 2014, 118, 27308-27317.	1.5	48
85	Atomistic investigation of the structure and transport properties of tilt grain boundaries of UO2. Journal of Nuclear Materials, 2015, 458, 45-55.	1.3	48
86	Water Adsorption on AnO₂ {111}, {110}, and {100} Surfaces (An = U and Pu): A Density Functional Theory + U Study. Journal of Physical Chemistry C, 2017, 121, 1675-1682.	1.5	48
87	Vibrational properties of CO on ceria surfaces. Surface Science, 2006, 600, 175-178.	0.8	46
88	Sorptive Characteristics of Organomontmorillonite toward Organic Compounds: A Combined LFERs and Molecular Dynamics Simulation Study. Environmental Science & Technology, 2011, 45, 6504-6510.	4.6	46
89	Ionic conductivity in nano-scale CeO2/YSZ heterolayers. Journal of Materials Chemistry, 2006, 16, 1067.	6.7	45
90	Elucidating the nature of grain boundary resistance in lithium lanthanum titanate. Journal of Materials Chemistry A, 2021, 9, 6487-6498.	5.2	44

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91	Surface Structures and Oxygen Hole Formation on the La2O3 Catalyst. A Computer Simulation Study. The Journal of Physical Chemistry, 1994, 98, 9637-9641.	2.9	43
92	Vacancy migration at the {410}/[001] symmetric tilt grain boundary of MgO: An atomistic simulation study. Physical Review B, 1997, 56, 11477-11484.	1.1	43
93	Proton-containing defects at forsterite {010} tilt grain boundaries and stepped surfaces. American Mineralogist, 2000, 85, 1143-1154.	0.9	43
94	Structure of Zeolite A (LTA) Surfaces and the Zeolite A/Water Interface. Journal of Physical Chemistry C, 2010, 114, 9739-9747.	1.5	43
95	Concurrent La and A-Site Vacancy Doping Modulates the Thermoelectric Response of SrTiO₃: Experimental and Computational Evidence. ACS Applied Materials & Interfaces, 2017, 9, 41988-42000.	4.0	43
96	Predicting the influence of growth additives on the morphology of ionic crystals. Journal of the Chemical Society Chemical Communications, 1991, , 1494.	2.0	42
97	Free Energy Change of Aggregation of Nanoparticles. Journal of Physical Chemistry C, 2008, 112, 14731-14736.	1.5	42
98	Mechanical properties of ceria nanorods and nanochains; the effect of dislocations, grain-boundaries and oriented attachment. Nanoscale, 2011, 3, 1823.	2.8	42
99	Ab Initio Investigation of the UO₃ Polymorphs: Structural Properties and Thermodynamic Stability. Inorganic Chemistry, 2014, 53, 12253-12264.	1.9	40
100	Free-energy calculations of thermodynamic, vibrational, elastic, and structural properties of Î±-quartz at variable pressures and temperatures. Physical Review B, 1996, 54, 826-835.	1.1	38
101	<scp>Group Status and Entrepreneurship</scp>. Journal of Economics and Management Strategy, 2010, 19, 919-945.	0.4	38
102	Impurity segregation to the surfaces of corundum-structured oxides. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 555.	1.1	37
103	Crystal structure and thermoelectric properties of Srâ€“Mo substituted CaMnO₃: a combined experimental and computational study. Journal of Materials Chemistry C, 2015, 3, 12245-12259.	2.7	37
104	Computer simulation of defect clusters in UO2 and their dependence on composition. Journal of Nuclear Materials, 2015, 456, 329-333.	1.3	37
105	Oxygen vacancy diffusion in alumina: New atomistic simulation methods applied to an old problem. Acta Materialia, 2009, 57, 4765-4772.	3.8	36
106	The Structure and Dynamics of Hydrated and Hydroxylated Magnesium Oxide Nanoparticles. Langmuir, 2011, 27, 1821-1829.	1.6	36
107	Dynamical instabilities in Î±-quartz and Î±-berlinite: A mechanism for amorphization. Physical Review B, 1995, 52, 13306-13309.	1.1	35
108	Density functional theory investigation of the layered uranium oxides U₃O₈ and U₂O₅. Dalton Transactions, 2015, 44, 2613-2622.	1.6	35

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109	Ab Initio Surface Phase Diagram of the {101Ì„4} Calcite Surface. Journal of Physical Chemistry B, 2005, 109, 18211-18213.	1.2	34
110	Atomistic simulation of the effect of temperature and pressure on the [001] symmetric tilt grain boundaries of MgO. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1996, 74, 407-418.	0.7	33
111	Computer modelling of metal - oxide interfaces. Journal of Physics Condensed Matter, 1997, 9, 5709-5717.	0.7	33
112	Atomistic simulation of charged iron oxyhydroxide surfaces in contact with aqueous solution. Chemical Communications, 2005, , 3027.	2.2	33
113	Atomistic Modeling of Multilayered Ceria Nanotubes. Nano Letters, 2007, 7, 543-546.	4.5	33
114	A Raman spectroscopic study of uranyl minerals from Cornwall, UK. RSC Advances, 2014, 4, 59137-59149.	1.7	33
115	The Shape of TiO₂-B Nanoparticles. Journal of the American Chemical Society, 2014, 136, 6306-6312.	6.6	33
116	Tuning Thermoelectric Properties of Misfit Layered Cobaltites by Chemically Induced Strain. Journal of Physical Chemistry C, 2015, 119, 21818-21827.	1.5	33
117	Atomistic simulation of the surface structure of electrolytic manganese dioxide. Surface Science, 2009, 603, 3184-3190.	0.8	32
118	Defect chemistry of Ti and Fe impurities and aggregates in Al2O3. Journal of Materials Chemistry A, 2014, 2, 6198-6208.	5.2	32
119	Atomistic simulation of screw dislocations in rock salt structured materials. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1999, 79, 527-536.	0.7	31
120	Negative compressibility in platinum sulfide using density-functional theory. Physical Review B, 2010, 81, .	1.1	31
121	Morphology and Surface Analysis of Pure and Doped Cuboidal Ceria Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 24561-24569.	1.5	31
122	Atomistic simulation of mineral surfaces: Studies of surface stability and growth. Phase Transitions, 1997, 61, 83-107.	0.6	30
123	Atomistic simulation of the effects of calcium and strontium defects on the surface structure and stability of BaSO4. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 1947-1952.	1.7	30
124	Atomistic simulation studies of magnetite surface structures and adsorption behavior in the presence of molecular and dissociated water and formic acid. Journal of Colloid and Interface Science, 2006, 295, 364-373.	5.0	30
125	Atomistic Simulation of the Surface Carbonation of Calcium and Magnesium Oxide Surfaces. Journal of Physical Chemistry C, 2009, 113, 8320-8328.	1.5	30
126	Comparison of atomistic simulations and pseudopotential calculations of the MgO{100}/Ag{100} and MgO{110}/Ag{110} interfaces. Journal of Chemical Physics, 1999, 110, 8090-8097.	1.2	29

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127	Modelling inorganic solids and their interfaces: A combined approach of atomistic and electronic structure simulation techniques. Faraday Discussions, 2003, 124, 155.	1.6	29
128	Atomistic Simulation of Yâ€Doped Î±â€Alumina Interfaces. Journal of the American Ceramic Society, 2008, 91, 3643-3651.	1.9	29
129	A computer simulation of the structure and elastic properties of MgSiO3 perovskite. Mineralogical Magazine, 1986, 50, 693-707.	0.6	28
130	Atomistic Modeling Study of Surface Segregation in Nd:YAG. Journal of the American Ceramic Society, 2006, 89, 3812-3816.	1.9	28
131	Living in the salt-cocrystal continuum: indecisive organic complexes with thermochromic behaviour. CrystEngComm, 2019, 21, 1626-1634.	1.3	28
132	Computer Simulation of Surface Segregation. Molecular Simulation, 1992, 9, 83-98.	0.9	27
133	The energetics of polytypic structures: a computer simulation of magnesium silicate spinelloids. Acta Crystallographica Section B: Structural Science, 1985, 41, 231-239.	1.8	26
134	Dopant control over the crystal morphology of ceramic materials. Surface Science, 2007, 601, 4793-4800.	0.8	26
135	Strongly Bound Surface Water Affects the Shape Evolution of Cerium Oxide Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 3577-3588.	1.5	26
136	Molecular dynamics simulation of fluoride-perovskites. Journal of Physics Condensed Matter, 1992, 4, 2097-2108.	0.7	25
137	Computer simulation of general grain boundaries in rocksalt oxides. Physical Review B, 1999, 60, 2740-2746.	1.1	25
138	Computer-Aided Design of Nanoceria Structures as Enzyme Mimetic Agents: The Role of Bodily Electrolytes on Maximizing Their Activity. ACS Applied Bio Materials, 2019, 2, 1098-1106.	2.3	25
139	Atomistic simulation methodologies for modelling the nucleation, growth and structure of interfaces. Journal of Materials Chemistry, 2000, 10, 1315-1324.	6.7	24
140	Atomistic simulation of the structure and segregation to the (0001) and surfaces of Fe2O3. Physics and Chemistry of Minerals, 2004, 31, 507-517.	0.3	24
141	Oxygen transport in unreduced, reduced and Rh(iii)-doped CeO2nanocrystals. Faraday Discussions, 2007, 134, 377-397.	1.6	24
142	Modelling the effects of surfactant loading level on the sorption of organic contaminants on organoclays. RSC Advances, 2015, 5, 47022-47030.	1.7	24
143	Elastic and nonlinear acoustic properties of the terbium iron garnetTb3Fe5O12in relation to those of other garnets. Physical Review B, 1992, 46, 8756-8767.	1.1	22
144	Atomistic simulation of the surface structure of wollastonite and adsorption phenomena relevant to flotation. International Journal of Mineral Processing, 2003, 72, 111-127.	2.6	22

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145	Computer aided design of nano-structured materials with tailored ionic conductivities. Physical Chemistry Chemical Physics, 2005, 7, 16.	1.3	22
146	Atomistic modelling of adsorption and segregation at inorganic solid interfaces. Molecular Simulation, 2009, 35, 584-608.	0.9	22
147	Atomistic Modeling of the Sorption Free Energy of Dioxins at Clayâ€“Water Interfaces. Journal of Physical Chemistry C, 2013, 117, 24975-24984.	1.5	22
148	Role of Structure and Defect Chemistry in High-Performance Thermoelectric Bismuth Strontium Cobalt Oxides. Chemistry of Materials, 2016, 28, 7470-7478.	3.2	22
149	Industrial Applications of Simulation Studies in Solid State Chemistry. Molecular Simulation, 1989, 3, 49-69.	0.9	21
150	Quartz amorphization: A dynamical instability. Philosophical Magazine Letters, 1995, 71, 59-64.	0.5	21
151	Atomistic Simulation of Surface Selectivity on Carbonate Formation at Calcium and Magnesium Oxide Surfaces. Journal of Physical Chemistry C, 2012, 116, 13240-13251.	1.5	21
152	Study of surfaces and morphologies of proteic solâ€“gel derived barium aluminate nanopowders: An experimental and computational study. Materials Chemistry and Physics, 2012, 136, 1052-1059.	2.0	21
153	Microscopic origin of the optical processes in blue sapphire. Chemical Communications, 2013, 49, 5259.	2.2	21
154	Some Observations on the Role of Dopants in Phase Transitions in Zirconia from Atomistic Simulations. Journal of the American Ceramic Society, 1990, 73, 3220-3224.	1.9	20
155	Atomistic simulation of the surface structure of wollastonite. Chemical Physics Letters, 2003, 377, 81-92.	1.2	20
156	Simulation of the Adsorption and Transport of CO2 on Faujasite Surfaces. Journal of Physical Chemistry C, 2013, 117, 21778-21787.	1.5	20
157	Effect of defects on the stability of heteroepitaxial ceramic interfaces studied by computer simulation. Physical Review B, 1994, 50, 14498-14505.	1.1	19
158	Atomistic Modeling of Gibbsite:Â Cation Incorporation. Journal of Physical Chemistry B, 2001, 105, 5099-5105.	1.2	19
159	Application of molecular dynamics DL_POLY codes to interfaces of inorganic materials. Molecular Simulation, 2006, 32, 1079-1093.	0.9	19
160	Surface and Mirror Twin Grain Boundary Segregation in Nd:YAG: An Atomistic Simulation Study. Journal of the American Ceramic Society, 2008, 91, 2698-2705.	1.9	19
161	Energy Minimization of Single-Walled Titanium Oxide Nanotubes. ACS Nano, 2009, 3, 3401-3412.	7.3	19
162	Lithium migration at low concentration in TiO 2 polymorphs. Computational and Theoretical Chemistry, 2015, 1072, 43-51.	1.1	19

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163	DL_MONTE: a multipurpose code for Monte Carlo simulation. Molecular Simulation, 2021, 47, 131-151.	0.9	19
164	Effect of Lattice Relaxation on Cation Exchange in Zeolite A Using Computer Simulation. Journal of Physical Chemistry B, 1997, 101, 9964-9972.	1.2	18
165	Atomistic simulation of crystal growth at the aã€ˆ100ã€‰ screw dislocation terminating at the {100} surface of MgO. Surface Science, 2001, 474, L185-L190.	0.8	18
166	Computer Simulation of Dissociative Adsorption of Water on the Surfaces of Spinel MgAl₂O₄. Journal of the American Ceramic Society, 2001, 84, 1553-1558.	1.9	17
167	Crystal morphology and surface structures of orthorhombic MgSiO3 perovskite. Physics and Chemistry of Minerals, 2005, 31, 671-682.	0.3	17
168	Competitive Adsorption on Wollastonite:Â An Atomistic Simulation Approach. Journal of Physical Chemistry B, 2005, 109, 11286-11295.	1.2	17
169	Hydride ion formation in stoichiometric UO₂. Chemical Communications, 2015, 51, 16209-16212.	2.2	17
170	Ba6â^'3x Nd8+2x Ti18O54 Tungsten Bronze: A New High-Temperature n-Type Oxide Thermoelectric. Journal of Electronic Materials, 2016, 45, 1894-1899.	1.0	17
171	The critical role of hydrogen on the stability of oxy-hydroxyl defect clusters in uranium oxide. Journal of Materials Chemistry A, 2018, 6, 11362-11369.	5.2	17
172	Accuracy of Hybrid Functionals with Non-Self-Consistent Kohnâ€“Sham Orbitals for Predicting the Properties of Semiconductors. Journal of Chemical Theory and Computation, 2020, 16, 3543-3557.	2.3	17
173	Information on catalyst surface structure from crystallite morphologies observed by scanning electron microscopy (SEM). Catalysis Letters, 1992, 15, 123-131.	1.4	16
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