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	Comparative Study of Oxygen Diffusion in Polyethylene Terephthalate and Polyethylene Furanoate Using Molecular Modeling: Computational Insights into the Mechanism for Gas Transport in Bulk Polymer Systems. Macromolecules, 2022, 55, 498-510.	2.2	14
2	Structural dynamics of Schottky and Frenkel defects in ThO₂: a density-functional theory study. Journal of Materials Chemistry A, 2022, 10, 1861-1875.	5.2	9
3	Surface chemistry and porosity engineering through etching reveal ultrafast oxygen reduction kinetics below 400ÂÂ°C in B-site exposed (La,Sr)(Co,Fe)O3 thin-films. Journal of Power Sources, 2022, 523, 230983.	4.0	8
4	SurfinPy 2.0: A Phase Diagram Generator for Surfaces and Bulk Phases. Journal of Open Source Software, 2022, 7, 4014.	2.0	1
5	Molecular simulation of hydrogen storage and transport in cellulose. Molecular Simulation, 2021, 47, 170-179.	0.9	3
6	DL_MONTE: a multipurpose code for Monte Carlo simulation. Molecular Simulation, 2021, 47, 131-151.	0.9	19
7	Elucidating the nature of grain boundary resistance in lithium lanthanum titanate. Journal of Materials Chemistry A, 2021, 9, 6487-6498.	5.2	44
8	Partially Anion-Ordered Cerium Niobium Oxynitride Perovskite Phase with a Small Band Gap. Chemistry of Materials, 2021, 33, 4045-4056.	3.2	1
9	Use of Interplay between Aâ€Site Nonâ€Stoichiometry and Hydroxide Doping to Deliver Novel Protonâ€Conducting Perovskite Oxides. Advanced Energy Materials, 2021, 11, 2101337.	10.2	11
10	Unraveling the Impact of Graphene Addition to Thermoelectric SrTiO₃ and La-Doped SrTiO₃ Materials: A Density Functional Theory Study. ACS Applied Materials & Interfaces, 2021, 13, 41303-41314.	4.0	14
11	Bacteriophage M13 Aggregation on a Microhole Poly(ethylene terephthalate) Substrate Produces an Anionic Current Rectifier: Sensitivity toward Anionic versus Cationic Guests. ACS Applied Bio Materials, 2020, 3, 512-521.	2.3	11
12	Thermodynamic Evolution of Cerium Oxide Nanoparticle Morphology Using Carbon Dioxide. Journal of Physical Chemistry C, 2020, 124, 23210-23220.	1.5	13
13	Quantifying the impact of disorder on Li-ion and Na-ion transport in perovskite titanate solid electrolytes for solid-state batteries. Journal of Materials Chemistry A, 2020, 8, 19603-19611.	5.2	15
14	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
15	The Atomic-Level Structure of Cementitious Calcium Aluminate Silicate Hydrate. Journal of the American Chemical Society, 2020, 142, 11060-11071.	6.6	107
16	The energetics of carbonated PuO₂ surfaces affects nanoparticle morphology: a DFT+U study. Physical Chemistry Chemical Physics, 2020, 22, 7728-7737.	1.3	8
17	Strongly Bound Surface Water Affects the Shape Evolution of Cerium Oxide Nanoparticles. Journal of Physical Chemistry C, 2020, 124, 3577-3588.	1.5	26
18	The usefulness of molecular-dynamics simulations in clarifying the activation enthalpy of oxygen-vacancy migration in the perovskite oxide BaTiO₃. Physical Chemistry Chemical Physics, 2020, 22, 5413-5417.	1.3	12

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19	Assessing molecular simulation for the analysis of lipid monolayer reflectometry. Journal of Physics Communications, 2019, 3, 075001.	0.5	9
20	Defect segregation facilitates oxygen transport at fluorite UO ₂ grain boundaries. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20190026.	1.6	12
21	The role of dopant segregation on the oxygen vacancy distribution and oxygen diffusion in CeO₂ grain boundaries *. JPhys Energy, 2019, 1, 042005.	2.3	12
22	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
23	Thermodynamics, Electronic Structure, and Vibrational Properties of Snn(S1â€“xSex)m Solid Solutions for Energy Applications. Chemistry of Materials, 2019, 31, 3672-3685.	3.2	11
24	Impact of Hydrogen on the Intermediate Oxygen Clusters and Diffusion in Fluorite Structured UO2+x. Inorganic Chemistry, 2019, 58, 3774-3779.	1.9	3
25	Bayesian determination of the effect of a deep eutectic solvent on the structure of lipid monolayers. Physical Chemistry Chemical Physics, 2019, 21, 6133-6141.	1.3	9
26	Living in the salt-cocrystal continuum: indecisive organic complexes with thermochromic behaviour. CrystEngComm, 2019, 21, 1626-1634.	1.3	28
27	surfinpy: A Surface Phase Diagram Generator. Journal of Open Source Software, 2019, 4, 1210.	2.0	7
28	An introduction to classical molecular dynamics simulation for experimental scattering users. Journal of Applied Crystallography, 2019, 52, 665-668.	1.9	3
29	Particle Morphology and Lithium Segregation to Surfaces of the Li₇La₃Zr₂O₁₂ Solid Electrolyte. Chemistry of Materials, 2018, 30, 3019-3027.	3.2	80
30	Prospects for Engineering Thermoelectric Properties in La_{1/3}NbO₃ Ceramics Revealed via Atomic-Level Characterization and Modeling. Inorganic Chemistry, 2018, 57, 45-55.	1.9	9
31	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
32	Combined EXAFS and ab initio study of copper complex geometries adsorbed on natural illite. Applied Clay Science, 2018, 152, 73-82.	2.6	3
33	Atomic-Level Characterization of Thermoelectric La1/3NbO3. Microscopy and Microanalysis, 2018, 24, 1534-1535.	0.2	0
34	The impact of tilt grain boundaries on the thermal transport in perovskite SrTiO₃ layered nanostructures. A computational study. Nanoscale, 2018, 10, 15010-15022.	2.8	14
35	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
36	pylj: A teaching tool for classical atomistic simulation. The Journal of Open Source Education, 2018, 1, 19.	0.2	2

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37	Carbonation of Hydrous Materials at the Molecular Level: A Time of Flight-Secondary Ion Mass Spectrometry, Raman and Density Functional Theory Study. Crystal Growth and Design, 2017, 17, 1036-1044.	1.4	16
38	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
39	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
40	Structure and Properties of Some Layered U₂O₅ Phases: A Density Functional Theory Study. Inorganic Chemistry, 2017, 56, 4468-4473.	1.9	16
41	Atomic-scale characterization of thermoelectric oxides using high spatial and energy resolution STEM-EELS. Microscopy and Microanalysis, 2017, 23, 370-371.	0.2	0
42	: A force field database for cementitious materials including validations, applications and opportunities. Cement and Concrete Research, 2017, 102, 68-89.	4.6	186
43	Structural, Electronic, and Transport Properties of Hybrid SrTiO₃-Graphene and Carbon Nanoribbon Interfaces. Chemistry of Materials, 2017, 29, 7364-7370.	3.2	14
44	A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor. Nature Communications, 2017, 8, 1800.	5.8	83
45	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
46	Nanostructuring perovskite oxides: the impact of SrTiO₃ nanocube 3D self-assembly on thermal conductivity. RSC Advances, 2016, 6, 114069-114077.	1.7	16
47	Role of Structure and Defect Chemistry in High-Performance Thermoelectric Bismuth Strontium Cobalt Oxides. Chemistry of Materials, 2016, 28, 7470-7478.	3.2	22
48	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.	7.8	447
49	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
50	An experimental and computational study to resolve the composition of dolomitic lime. RSC Advances, 2016, 6, 16066-16072.	1.7	8
51	Observation of a re-entrant phase transition in the molecular complex tris(Î¼₂-3,5-diisopropyl-1,2,4-triazolato-Îº²N¹:N²)trigold(I) under high pressure. IUCrJ, 2016, 3, 367-376.	2.0	6
52	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, .	3.7	133
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	A Giant Reconstruction of Î±-quartz (0001) Interpreted as Three Domains of Nano Dauphine Twins. Scientific Reports, 2015, 5, 14545.	1.6	11

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55	Toward Knowledgeâ€Based Grainâ€Boundary Engineering of Transparent Alumina Combining Advanced <scp>TEM</scp> and Atomistic Modeling. Journal of the American Ceramic Society, 2015, 98, 1959-1964.	1.9	9
56	Density functional theory calculations of defective UO2 at U3O7 stoichiometry. Journal of Nuclear Materials, 2015, 467, 724-729.	1.3	16
57	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
58	High-Temperature Thermoelectric Properties of (1Ââ^'Âx) SrTiO3Ââ^'Â(x) La1/3NbO3 Ceramic Solid Solution. Journal of Electronic Materials, 2015, 44, 1803-1808.	1.0	14
59	Modelling the effects of surfactant loading level on the sorption of organic contaminants on organoclays. RSC Advances, 2015, 5, 47022-47030.	1.7	24
60	Density functional theory investigation of the layered uranium oxides U₃O₈ and U₂O₅. Dalton Transactions, 2015, 44, 2613-2622.	1.6	35
61	Energetics, thermal isomerisation and photochemistry of the linkage-isomer system [Ni(Et₄dien)(Î·²-O,ON)(Î·¹-NO₂)]. CrystEngComm, 2015, 17, 383-394.	1.3	16
62	Interfacial Electron-Shuttling Processes across KolliphorEL Monolayer Grafted Electrodes. ACS Applied Materials & Interfaces, 2015, 7, 15458-15465.	4.0	10
63	Hydride ion formation in stoichiometric UO₂. Chemical Communications, 2015, 51, 16209-16212.	2.2	17
64	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
65	Electronic excitations in molecular solids: bridging theory and experiment. Faraday Discussions, 2015, 177, 181-202.	1.6	11
66	Tuning Thermoelectric Properties of Misfit Layered Cobaltites by Chemically Induced Strain. Journal of Physical Chemistry C, 2015, 119, 21818-21827.	1.5	33
67	Lithium migration at low concentration in TiO 2 polymorphs. Computational and Theoretical Chemistry, 2015, 1072, 43-51.	1.1	19
68	Computer simulation of defect clusters in UO2 and their dependence on composition. Journal of Nuclear Materials, 2015, 456, 329-333.	1.3	37
69	A Raman spectroscopic study of uranyl minerals from Cornwall, UK. RSC Advances, 2014, 4, 59137-59149.	1.7	33
70	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
71	Mechanical properties of mesoporous ceria nanoarchitectures. Physical Chemistry Chemical Physics, 2014, 16, 24899-24912.	1.3	3
72	Ab Initio Investigation of the UO₃ Polymorphs: Structural Properties and Thermodynamic Stability. Inorganic Chemistry, 2014, 53, 12253-12264.	1.9	40

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73	The Shape of TiO₂-B Nanoparticles. Journal of the American Chemical Society, 2014, 136, 6306-6312.	6.6	33
74	Defect chemistry of Ti and Fe impurities and aggregates in Al2O3. Journal of Materials Chemistry A, 2014, 2, 6198-6208.	5.2	32
75	Particle shapes and surface structures of olivine NaFePO₄ in comparison to LiFePO₄. Physical Chemistry Chemical Physics, 2014, 16, 21788-21794.	1.3	61
76	Surface properties of Î±-MnO₂: relevance to catalytic and supercapacitor behaviour. Journal of Materials Chemistry A, 2014, 2, 15509-15518.	5.2	121
77	Structural, electronic and thermoelectric behaviour of CaMnO₃ and CaMnO_(3â^'Î). Journal of Materials Chemistry A, 2014, 2, 14109-14117.	5.2	98
78	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
79	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. Physical Review B, 2014, 89, .	1.1	212
80	DL_MONTE: a general purpose program for parallel Monte Carlo simulation. Molecular Simulation, 2013, 39, 1240-1252.	0.9	66
81	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
82	Simulation of the Adsorption and Transport of CO2 on Faujasite Surfaces. Journal of Physical Chemistry C, 2013, 117, 21778-21787.	1.5	20
83	Microscopic origin of the optical processes in blue sapphire. Chemical Communications, 2013, 49, 5259.	2.2	21
84	Monte Carlo simulation and free energies of mixed oxide nanoparticles. Physical Chemistry Chemical Physics, 2013, 15, 6219.	1.3	5
85	Nanostructuring of Î²-MnO₂: The Important Role of Surface to Bulk Ion Migration. Chemistry of Materials, 2013, 25, 536-541.	3.2	99
86	Environment-mediated structure, surface redox activity and reactivity of ceria nanoparticles. Nanoscale, 2013, 5, 6063.	2.8	71
87	Morphology and Surface Analysis of Pure and Doped Cuboidal Ceria Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 24561-24569.	1.5	31
88	Modeling the Interaction of Nanoparticles with Mineral Surfaces: Adsorbed C₆₀ on Pyrophyllite. Journal of Physical Chemistry A, 2013, 117, 6602-6611.	1.1	15
89	Cationic Surface Reconstructions on Cerium Oxide Nanocrystals: An Aberration-Corrected HRTEM Study. ACS Nano, 2012, 6, 421-430.	7.3	53
90	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

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91	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
92	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
93	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
94	Mechanical properties of ceria nanorods and nanochains; the effect of dislocations, grain-boundaries and oriented attachment. Nanoscale, 2011, 3, 1823.	2.8	42
95	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
96	The Structure and Dynamics of Hydrated and Hydroxylated Magnesium Oxide Nanoparticles. Langmuir, 2011, 27, 1821-1829.	1.6	36
97	Structural characterization of amorphous alumina and its polymorphs from first-principles XPS and NMR calculations. Physical Review B, 2011, 83, .	1.1	90
98	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
99	Electron hopping rate measurements in ITO junctions: Charge diffusion in a layer-by-layer deposited ruthenium(II)-bis(benzimidazolyl)pyridine-phosphonateâ€“TiO2 film. Journal of Electroanalytical Chemistry, 2011, 657, 196-201.	1.9	13
100	ElAM: A computer program for the analysis and representation of anisotropic elastic properties. Computer Physics Communications, 2010, 181, 2102-2115.	3.0	321
101	Growth modification of seeded calcite using carboxylic acids: Atomistic simulations. Journal of Colloid and Interface Science, 2010, 346, 226-231.	5.0	63
102	<scp>Group Status and Entrepreneurship</scp>. Journal of Economics and Management Strategy, 2010, 19, 919-945.	0.4	38
103	Negative compressibility in platinum sulfide using density-functional theory. Physical Review B, 2010, 81, .	1.1	31
104	Structure of Zeolite A (LTA) Surfaces and the Zeolite A/Water Interface. Journal of Physical Chemistry C, 2010, 114, 9739-9747.	1.5	43
105	Lithium Coordination Sites in Li_xTiO₂(B): A Structural and Computational Study. Chemistry of Materials, 2010, 22, 6426-6432.	3.2	104
106	Oxygen vacancy diffusion in alumina: New atomistic simulation methods applied to an old problem. Acta Materialia, 2009, 57, 4765-4772.	3.8	36
107	Atomistic simulation of the surface structure of electrolytic manganese dioxide. Surface Science, 2009, 603, 3184-3190.	0.8	32
108	Lithium Insertion and Transport in the TiO₂â^'B Anode Material: A Computational Study. Chemistry of Materials, 2009, 21, 4778-4783.	3.2	169

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109	Atomistic Simulation of the Surface Carbonation of Calcium and Magnesium Oxide Surfaces. Journal of Physical Chemistry C, 2009, 113, 8320-8328.	1.5	30
110	Energy Minimization of Single-Walled Titanium Oxide Nanotubes. ACS Nano, 2009, 3, 3401-3412.	7.3	19
111	Atomistic modelling of adsorption and segregation at inorganic solid interfaces. Molecular Simulation, 2009, 35, 584-608.	0.9	22
112	eScience for molecular-scale simulations and the e Minerals project. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 967-985.	1.6	8
113	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
114	Atomistic Simulation of Yâ€Ðoped Î±â€Alumina Interfaces. Journal of the American Ceramic Society, 2008, 91, 3643-3651.	1.9	29
115	Free Energy Change of Aggregation of Nanoparticles. Journal of Physical Chemistry C, 2008, 112, 14731-14736.	1.5	42
116	Low-energy surface phonons onÎ±-quartz (0001). Physical Review B, 2008, 78, .	1.1	8
117	Electrostatic versus polarization effects in the adsorption of aromatic molecules of varied polarity on an insulating hydrophobic surface. Journal of Physics Condensed Matter, 2008, 20, 035215.	0.7	16
118	Molecular Simulation of Mineral Surfaces and the Role of Impurities on Surface Stability. AIP Conference Proceedings, 2007, , .	0.3	2
119	Oxygen transport in unreduced, reduced and Rh(iii)-doped CeO2nanocrystals. Faraday Discussions, 2007, 134, 377-397.	1.6	24
120	Atomistic Modeling of Multilayered Ceria Nanotubes. Nano Letters, 2007, 7, 543-546.	4.5	33
121	Dopant control over the crystal morphology of ceramic materials. Surface Science, 2007, 601, 4793-4800.	0.8	26
122	Reduction of NO2on Ceria Surfaces. Journal of Physical Chemistry B, 2006, 110, 2256-2262.	1.2	117
123	Application of molecular dynamics DL_POLY codes to interfaces of inorganic materials. Molecular Simulation, 2006, 32, 1079-1093.	0.9	19
124	CeO2catalysed conversion of CO, NO2and NO from first principles energetics. Physical Chemistry Chemical Physics, 2006, 8, 216-218.	1.3	107
125	Information Delivery in Computational Mineral Science: The eMinerals Data Handling System. , 2006, , .		1
126	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

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127	Molecular Dynamics Simulations of Electrolyte Solutions at the (100) Goethite Surface. Journal of Physical Chemistry B, 2006, 110, 20491-20501.	1.2	54
128	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
129	Ionic conductivity in nano-scale CeO2/YSZ heterolayers. Journal of Materials Chemistry, 2006, 16, 1067.	6.7	45
130	Atomistic Modeling Study of Surface Segregation in Nd:YAG. Journal of the American Ceramic Society, 2006, 89, 3812-3816.	1.9	28
131	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
132	Vibrational properties of CO on ceria surfaces. Surface Science, 2006, 600, 175-178.	0.8	46
133	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
134	Computer Modelling of Oxygen Mobility at Ceria Surfaces and the Construction of Ceria Nanotube Models. Advances in Science and Technology, 2006, 46, 48.	0.2	0
135	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
136	The electronic structure of oxygen vacancy defects at the low index surfaces of ceria. Surface Science, 2005, 595, 223-232.	0.8	690
137	Crystal morphology and surface structures of orthorhombic MgSiO3 perovskite. Physics and Chemistry of Minerals, 2005, 31, 671-682.	0.3	17
138	Crystal morphology and surface structures of orthorhombic MgSiO3 in the presence of divalent impurity ions. Physics and Chemistry of Minerals, 2005, 32, 379-387.	0.3	6
139	TheeMinerals collaboratory: tools and experience. Molecular Simulation, 2005, 31, 329-337.	0.9	4
140	Atomistic simulation of charged iron oxyhydroxide surfaces in contact with aqueous solution. Chemical Communications, 2005, , 3027.	2.2	33
141	Oxidising CO to CO2 using ceria nanoparticles. Physical Chemistry Chemical Physics, 2005, 7, 2936.	1.3	159
142	Competitive Adsorption on Wollastonite:Â An Atomistic Simulation Approach. Journal of Physical Chemistry B, 2005, 109, 11286-11295.	1.2	17
143	Computer aided design of nano-structured materials with tailored ionic conductivities. Physical Chemistry Chemical Physics, 2005, 7, 16.	1.3	22
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145	Molecular dynamics simulations of the interactions between water and inorganic solids. Journal of Materials Chemistry, 2005, 15, 1454.	6.7	95
146	Ab Initio Surface Phase Diagram of the {101Ì„4} Calcite Surface. Journal of Physical Chemistry B, 2005, 109, 18211-18213.	1.2	34
147	Electronic structure of the antiferromagneticB1-structured FeO. Physical Review B, 2004, 70, .	1.1	57
148	High-temperature structure and dynamics of coesite (SiO2) from numerical simulations. Physics and Chemistry of Minerals, 2004, 31, 569-579.	0.3	16
149	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
150	Modelling Inorganic Solids and Their Interfaces: A Combined Approach of Atomistic and Electronic Structure Simulation Techniques. ChemInform, 2004, 35, no.	0.1	1
151	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
152	Ab initiomorphology and surface thermodynamics ofÎ±â˜Al2O3. Physical Review B, 2004, 69, .	1.1	117
153	From HADES to PARADISEâ€"atomistic simulation of defects in minerals. Journal of Physics Condensed Matter, 2004, 16, S2735-S2749.	0.7	9
154	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
155	Shape of CeO2 nanoparticles using simulated amorphisation and recrystallisation. Chemical Communications, 2004, , 2438.	2.2	84
156	Atomistic simulation of the surface structure of wollastonite. Chemical Physics Letters, 2003, 377, 81-92.	1.2	20
157	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
158	Modelling inorganic solids and their interfaces: A combined approach of atomistic and electronic structure simulation techniques. Faraday Discussions, 2003, 124, 155.	1.6	29
159	Atomistic Simulation of the Dissociative Adsorption of Water on Calcite Surfaces. Journal of Physical Chemistry B, 2003, 107, 7676-7682.	1.2	141
160	Synthesis, structure and ionic conductivity in nanopolycrystalline BaF2/CaF2 heterolayersElectronic supplementary information (ESI) available: potential parameters and pertinent calculated physical properties for the perfect BaF2 and CaF2. See http://www.rsc.org/suppdata/cc/b3/b305393h/. Chemical Communications, 2003, , 1804.	2.2	15
161	Metal oxide encapsulated nanoparticles. Journal of Materials Chemistry, 2003, 13, 2078.	6.7	5
162	Calculating the vibrational thermodynamic properties of bulk oxides using lattice dynamics and molecular dynamics. Physical Review B, 2003, 67, .	1.1	14

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163	Encapsulated Oxide Nanoparticles:Â The Influence of the Microstructure on Associated Impurities within a Material. Journal of the American Chemical Society, 2003, 125, 8581-8588.	6.6	14
164	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.	0.9	12
165	Modelling the effect of water on cation exchange in zeolite A. Journal of Materials Chemistry, 2002, 12, 124-131.	6.7	84
166	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
167	Surfaceâ€“water interactions in the dolomite problem. Physical Chemistry Chemical Physics, 2001, 3, 3217-3221.	1.3	79
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