Graeme W Watson

List of Publications by Citations

218 papers	15,367 citations	64 h-index	119 g-index
232 ext. papers	16,599 ext. citations	5.1 avg, IF	6.76 L-index

#	Paper	IF	Citations
218	Band alignment of rutile and anatase TiO*Nature Materials*, **2013**, 12, 798-801	27	1656
217	The electronic structure of oxygen vacancy defects at the low index surfaces of ceria. *Surface Science*, **2005**, 595, 223-232	1.8	585
216	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	1.8	576
215	Stereochemistry of post-transition metal oxides: revision of the classical lone pair model. *Chemical Society Reviews*, **2011**, 40, 4455-63	58.5	456
214	Theoretical and Experimental Study of the Electronic Structures of MoO3 and MoO2. *Journal of Physical Chemistry C*, **2010**, 114, 4636-4645	3.8	435
213	A DFT+U description of oxygen vacancies at the TiO2 rutile (110) surface. *Surface Science*, **2007**, 601, 5034-5041	1.8	410
212	Atomistic simulation of dislocations, surfaces and interfaces in MgO. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 433		374
211	Intrinsic n-type Defect Formation in TiO2: A Comparison of Rutile and Anatase from GGA+U Calculations. *Journal of Physical Chemistry C*, **2010**, 114, 2321-2328	3.8	326
210	Atomistic simulation of the surface structure of theTiO2 polymorphs rutileand anatase. *Journal of Materials Chemistry*, **1997**, 7, 563-568		278
209	Oxygen vacancy formation and migration in ceria. *Solid State Ionics*, **2006**, 177, 3069-3074	3.3	256
208	Acceptor levels in p-type Cu(2)O: rationalizing theory and experiment. *Physical Review Letters*, **2009** , 103, 096405	7.4	237
207	Energetic and Electronic Structure Analysis of Intrinsic Defects in SnO2. *Journal of Physical Chemistry C*, **2009**, 113, 439-448	3.8	236
206	Polaronic trapping of electrons and holes by native defects in anatase TiO2. *Physical Review B*, **2009** , 80,	3.3	222
205	Atomistic models for CeO(2)(111), (110), and (100) nanoparticles, supported on yttrium-stabilized zirconia. *Journal of the American Chemical Society*, **2002**, 124, 11429-39	16.4	213
204	The origin of the stereochemically active Pb(II) lone pair: DFT calculations on PbO and PbS. *Journal of Solid State Chemistry*, **2005**, 178, 1422-1428	3.3	207
203	A Density Functional Theory + U Study of Oxygen Vacancy Formation at the (110), (100), (101), and (001) Surfaces of Rutile TiO2. *Journal of Physical Chemistry C*, **2009**, 113, 7322-7328	3.8	192
202	Electronic origins of structural distortions in post-transition metal oxides: experimental and theoretical evidence for a revision of the lone pair model. *Physical Review Letters*, **2006**, 96, 157403	7.4	182

201	An ab initio Study of Reduction of V2O5 through the Formation of Oxygen Vacancies and Li Intercalation. *Journal of Physical Chemistry C*, **2008**, 112, 9903-9911	3.8	181
200	Electronic structure of the □and □phases of Bi2O3: A combined ab initio and x-ray spectroscopy study. *Physical Review B*, **2006**, 73,	3.3	168
199	A Comparison of the Adsorption and Diffusion of Hydrogen on the {111} Surfaces of Ni, Pd, and Pt from Density Functional Theory Calculations. *Journal of Physical Chemistry B*, **2001**, 105, 4889-4894	3.4	168
198	Understanding the p-type defect chemistry of CuCrO2. *Journal of Materials Chemistry*, **2011**, 21, 3655		163
197	Role of Lattice Distortions in the Oxygen Storage Capacity of Divalently Doped CeO2. *Chemistry of Materials*, **2011**, 23, 4464-4468	9.6	158
196	The surface dependence of CO adsorption on Ceria. *Journal of Physical Chemistry B*, **2006**, 110, 16600-6	3.4	157
195	Sources of conductivity and doping limits in CdO from hybrid density functional theory. *Journal of the American Chemical Society*, **2011**, 133, 15065-72	16.4	149
194	Influence of the anion on lone pair formation in Sn(II) monochalcogenides: a DFT study. *Journal of Physical Chemistry B*, **2005**, 109, 18868-75	3.4	149
193	Ab initio calculation of the origin of the distortion of □PbO. *Physical Review B*, **1999**, 59, 8481-8486	3.3	146
192	Origin of the Lone Pair of □PbO from Density Functional Theory Calculations. *Journal of Physical Chemistry B*, **1999**, 103, 1258-1262	3.4	144
191	Small polarons in Nb- and Ta-doped rutile and anatase TiO2. *Journal of Materials Chemistry*, **2009**, 19, 5175		143
190	On the possibility of p-type SnO2. *Journal of Materials Chemistry*, **2012**, 22, 25236		134
189	Analysis of Intrinsic Defects in CeO2 Using a Koopmans-Like GGA+U Approach. *Journal of Physical Chemistry C*, **2012**, 116, 2443-2452	3.8	125
188	Reduction of NO2 on ceria surfaces. *Journal of Physical Chemistry B*, **2006**, 110, 2256-62	3.4	115
187	Modeling the polaronic nature of p-type defects in Cu2O: the failure of GGA and GGA + U. *Journal of Chemical Physics*, **2009**, 131, 124703	3.9	113
186	Undoped n-Type Cu2O: Fact or Fiction?. *Journal of Physical Chemistry Letters*, **2010**, 1, 2582-2585	6.4	111
185	Origin of the Bipolar Doping Behavior of SnO from X-ray Spectroscopy and Density Functional Theory. *Chemistry of Materials*, **2013**, 25, 3114-3123	9.6	107
184	Occupation matrix control of d- and f-electron localisations using DFT + U. *Physical Chemistry Chemical Physics*, **2014**, 16, 21016-31	3.6	105

183	Electronic structures of rocksalt, litharge, and herzenbergite SnO by density functional theory. *Physical Review B*, **2004**, 70,	3.3	105
182	Conductivity Limits in CuAlO2 from Screened-Hybrid Density Functional Theory. *Journal of Physical Chemistry Letters*, **2010**, 1, 3195-3199	6.4	102
181	Effect of Cr substitution on the electronic structure of CuAl1⊠CrxO2. *Physical Review B*, **2009**, 79,	3.3	102
180	Hole localization in Al doped silica: A DFT + U description. *Journal of Chemical Physics*, **2006**, 125, 144701	3.9	101
179	CeO2 catalysed conversion of CO, NO2 and NO from first principles energetics. *Physical Chemistry Chemical Physics*, **2006**, 8, 216-8	3.6	98
178	Understanding conductivity anomalies in Cu(I)-based delafossite transparent conducting oxides: Theoretical insights. *Journal of Chemical Physics*, **2010**, 132, 024707	3.9	93
177	GGA+U description of lithium intercalation into anatase TiO2. *Physical Review B*, **2010**, 82,	3.3	93
176	Experimental and theoretical study of the electronic structures of ⊞PbO and ⊞PbO2. *Journal of Materials Chemistry*, **2007**, 17, 267-277		92
175	Oxygen Vacancy Ordering and the Conductivity Maximum in Y2O3-Doped CeO2. *Chemistry of Materials*, **2012**, 24, 222-229	9.6	91
174	Surface Sensitivity in Lithium-Doping of MgO: A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. *Journal of Physical Chemistry C*, **2007**, 111, 7971-7979	3.8	91
173	Understanding the p-Type Conduction Properties of the Transparent Conducting Oxide CuBO2: A Density Functional Theory Analysis. *Chemistry of Materials*, **2009**, 21, 4568-4576	9.6	89
172	Geometry, Electronic Structure, and Bonding in CuMCh2(M = Sb, Bi; Ch = S, Se): Alternative Solar Cell Absorber Materials?. *Journal of Physical Chemistry C*, **2012**, 116, 7334-7340	3.8	87
171	Defect chemistry and surface properties ofLaCoO3. *Journal of Materials Chemistry*, **2000**, 10, 2298-2305		87
170	The origin of the electron distribution in SnO. *Journal of Chemical Physics*, **2001**, 114, 758	3.9	86
169	The recognition and sensing of anions through "positive allosteric effects" using simple urea-amide receptors. *Journal of Organic Chemistry*, **2008**, 73, 9235-44	4.2	83
168	Interface stoichiometry control to improve device voltage and modify band alignment in ZnO/Cu2O heterojunction solar cells. *Energy and Environmental Science*, **2014**, 7, 3606-3610	35.4	82
167	X-ray spectroscopic study of the electronic structure of CuCrO2. *Physical Review B*, **2009**, 79,	3.3	82
166	Solution Processing Route to Multifunctional Titania Thin Films: Highly Conductive and Photcatalytically Active Nb:TiO2. *Advanced Functional Materials*, **2014**, 24, 5075-5085	15.6	81

165	Tin Monoxide: Structural Prediction from First Principles Calculations with van der Waals Corrections. *Journal of Physical Chemistry C*, **2011**, 115, 19916-19924	3.8	79
164	Convergence of density and hybrid functional defect calculations for compound semiconductors. *Physical Review B*, **2013**, 88,	3.3	77
163	Evidence and Effect of Photogenerated Charge Transfer for Enhanced Photocatalysis in WO3/TiO2 Heterojunction Films: A Computational and Experimental Study. *Advanced Functional Materials*, **2017**, 27, 1605413	15.6	76
162	Nature of the band gap and origin of the conductivity of PbO2 revealed by theory and experiment. *Physical Review Letters*, **2011**, 107, 246402	7.4	76
161	Molecular-dynamics simulations of nickel oxide surfaces. *Physical Review B*, **1995**, 52, 5323-5329	3.3	76
160	Atomistic simulation of the surface structure of spinel. *Journal of Materials Chemistry*, **1994**, 4, 813		76
159	Density functional theory calculations of adsorption of water at calcium oxide and calcium fluoride surfaces. *Surface Science*, **2000**, 452, 9-19	1.8	75
158	The origin of the enhanced oxygen storage capacity of Ce(1-x)(Pd/Pt)(x)O2. *Physical Chemistry Chemical Physics*, **2011**, 13, 4279-84	3.6	74
157	The electronic structure of the antimony chalcogenide series: Prospects for optoelectronic applications. *Journal of Solid State Chemistry*, **2014**, 213, 116-125	3.3	68
156	Tracking DNA Excited States by Picosecond-Time-Resolved Infrared Spectroscopy: Signature Band for a Charge-Transfer Excited State in Stacked Adenine□Thymine Systems. *Journal of Physical Chemistry Letters*, **2013**, 4, 2739-2744	6.4	68
155	(Cu2S2)(Sr3Sc2O5)□ A Layered, Direct Band Gap, p-Type Transparent Conducting Oxychalcogenide: A Theoretical Analysis.. *Chemistry of Materials*, **2009**, 21, 5435-5442	9.6	66
154	Electronic structure of mixed-valence silver oxide AgO from hybrid density-functional theory. *Physical Review B*, **2010**, 81,	3.3	64
153	Computer simulation of the structure and stability of forsterite surfaces. *Physics and Chemistry of Minerals*, **1997**, 25, 70-78	1.6	64
152	Surface structures and defect properties of pure and doped La2NiO4. *Journal of Materials Chemistry*, **2001**, 11, 2597-2602		64
151	Reactivity on the (110) Surface of Ceria: A GGA+U Study of Surface Reduction and the Adsorption of CO and NO2. *Journal of Physical Chemistry C*, **2009**, 113, 11095-11103	3.8	63
150	Electronic Structures of Antimony Oxides. *Journal of Physical Chemistry C*, **2013**, 117, 14759-14769	3.8	62
149	Charge localization increases chemical expansion in cerium-based oxides. *Physical Chemistry Chemical Physics*, **2012**, 14, 12070-4	3.6	61
148	Elucidating the Nature of Pseudo Jahn□Teller Distortions in LixMnPO4: Combining Density Functional Theory with Soft and Hard X-ray Spectroscopy. *Journal of Physical Chemistry C*, **2013**, 117, 10383-10396	3.8	61

147	Ceria co-doping: synergistic or average effect?. *Physical Chemistry Chemical Physics*, **2014**, 16, 8320-31	3.6	60
146	Band gap anomalies of the ZnM2(III)O4 (M(III)=Co, Rh, Ir) spinels. *Physical Chemistry Chemical Physics*, **2011**, 13, 9667-75	3.6	60
145	Understanding the defect chemistry of tin monoxide. *Journal of Materials Chemistry C*, **2013**, 1, 8194	7.1	59
144	Why is lead dioxide metallic?. *Chemical Physics Letters*, **2005**, 411, 181-185	2.5	59
143	Cu3MCh3 (M = Sb, Bi; Ch = S, Se) as candidate solar cell absorbers: insights from theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 15477-84	3.6	58
142	The electronic structure of alkali doped alkaline earth metal oxides: Li doping of MgO studied with DFT-GGA and GGA+U. *Surface Science*, **2005**, 586, 25-37	1.8	57
141	Simulation of the structure and stability of sphalerite (ZnS) surfaces. *American Mineralogist*, **1998**, 83, 141-146	2.9	53
140	Electronic structures of silver oxides. *Physical Review B*, **2011**, 84,	3.3	51
139	Valence-band density of states and surface electron accumulation in epitaxial SnO2 films. *Physical Review B*, **2014**, 90,	3.3	50
138	Asymmetric acyl-transfer promoted by readily assembled chiral 4-N,N-dialkylaminopyridine derivatives. *Organic and Biomolecular Chemistry*, **2006**, 4, 2785-93	3.9	50
137	Microwave induced preparation of a-axis oriented double-ended needle-shaped ZnO microparticles. *Chemical Communications*, **2004**, 2294-5	5.8	50
136	Structure and Reducibility of CeO2 Doped with Trivalent Cations. *Journal of Physical Chemistry C*, **2016**, 120, 23430-23440	3.8	49
135	Experimental and theoretical study of the electronic structure of HgO and Tl2O3. *Physical Review B*, **2005**, 71,	3.3	48
134	Uncovering the complex behavior of hydrogen in Cu2O. *Physical Review Letters*, **2011**, 106, 186403	7.4	46
133	Understanding doping anomalies in degenerate p-type semiconductor LaCuOSe. *Journal of Materials Chemistry C*, **2014**, 2, 3429-3438	7.1	45
132	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		45
131	Vibrational properties of CO on ceria surfaces. *Surface Science*, **2006**, 600, 175-178	1.8	42
130	Reducing the chemical expansion coefficient in ceria by addition of zirconia. *Energy and Environmental Science*, **2013**, 6, 1142	35.4	40

129	Cooperative Mechanism for the Diffusion of Li+ Ions in LiMgSO4F. *Journal of Physical Chemistry C*, **2012**, 116, 18618-18625	3.8	40
128	Polymorphism in Bismuth Stannate: A First-Principles Study. *Chemistry of Materials*, **2007**, 19, 5158-5164	9.6	40
127	Understanding conductivity in SrCu2O2: stability, geometry and electronic structure of intrinsic defects from first principles. *Journal of Materials Chemistry*, **2010**, 20, 1086-1096		39
126	A comparative picosecond transient infrared study of 1-methylcytosine and 5'-dCMP that sheds further light on the excited states of cytosine derivatives. *Journal of the American Chemical Society*, **2011**, 133, 4212-5	16.4	39
125	Density Functional Theory Calculations on the Interaction of Ethene with the {111} Surface of Platinum. *Journal of Physical Chemistry B*, **2000**, 104, 6439-6446	3.4	39
124	Methanol conversion to hydrocarbons over zeolite catalysts: comments on the reaction mechanism for the formation of the first carbon□carbon bond. *Microporous and Mesoporous Materials*, **1999**, 29, 67-77	5.3	39
123	Role of Lithium Ordering in the LixTiO2 Anatase -> Titanate Phase Transition. *Journal of Physical Chemistry Letters*, **2011**, 2, 1657-1661	6.4	38
122	Ultrafast IR spectroscopy of the short-lived transients formed by UV excitation of cytosine derivatives. *Chemical Communications*, **2007**, 2130-2	5.8	38
121	Validation of all-atom phosphatidylcholine lipid force fields in the tensionless NPT ensemble. *Biochimica Et Biophysica Acta - Biomembranes*, **2009**, 1788, 638-49	3.8	37
120	Nature of the band gap of Tl2O3. *Physical Review B*, **2011**, 83,	3.3	37
119	Nature of electronic states at the Fermi level of metallic □bO2 revealed by hard x-ray photoemission spectroscopy. *Physical Review B*, **2007**, 75,	3.3	36
118	Hydrogen adsorption and diffusion on Pt {111} and PtSn {111}. *Journal of Materials Chemistry*, **2006**, 16, 1989		36
117	Vacancy migration at the {410}/[001] symmetric tilt grain boundary of MgO: An atomistic simulation study. *Physical Review B*, **1997**, 56, 11477-11484	3.3	35
116	Intrinsic ferromagnetism in CeO(2): dispelling the myth of vacancy site localization mediated superexchange. *Journal of Physics Condensed Matter*, **2009**, 21, 405502	1.8	34
115	Free-energy calculations of thermodynamic, vibrational, elastic, and structural properties of alpha -quartz at variable pressures and temperatures. *Physical Review B*, **1996**, 54, 826-835	3.3	34
114	The electronic structure of sulvanite structured semiconductors Cu3MCh4 (M = V, Nb, Ta; Ch = S, Se, Te): prospects for optoelectronic applications. *Journal of Materials Chemistry C*, **2015**, 3, 12236-12244	7.1	33
113	Comparative study of bandwidths in copper delafossites from x-ray emission spectroscopy. *Physical Review B*, **2009**, 80,	3.3	33
112	Aggregation induced emission (AIE) active 4-amino-1,8-naphthalimide-Tr□er's base for the selective sensing of chemical explosives in competitive aqueous media. *Chemical Communications*, **2020**, 56, 2562-2565	5.8	32

111	Atomistic modeling of multilayered ceria nanotubes. *Nano Letters*, **2007**, 7, 543-6	11.5	32
110	Oxidation of thioethers and sulfoxides with hydrogen peroxide using TS-1 as catalyst. *Physical Chemistry Chemical Physics*, **2000**, 2, 1523-1529	3.6	32
109	Dynamical instabilities in alpha -quartz and alpha -berlinite: A mechanism for amorphization. *Physical Review B*, **1995**, 52, 13306-13309	3.3	32
108	Computational testing of trivalent dopants in CeO2 for improved high-κ dielectric behaviour. *Journal of Materials Chemistry C*, **2013**, 1, 1093-1098	7.1	30
107	A GGA+U study of the reduction of ceria surfaces and their partial reoxidation through NO2 adsorption. *Molecular Simulation*, **2009**, 35, 577-583	2	30
106	Synthesis, structural characterisation and antiproliferative activity of a new fluorescent 4-amino-1,8-naphthalimide Tröger's base-Ru(ii)-curcumin organometallic conjugate. *Chemical Communications*, **2018**, 54, 4120-4123	5.8	29
105	Ab initio simulation of the interaction of hydrogen with the {111} surfaces of platinum, palladium and nickel. A possible explanation for their difference in hydrogenation activity. *Chemical Communications*, **2000**, 705-706	5.8	29
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103	The synthesis and characterisation of novel ferrocenyl polyphenylenes. *Dalton Transactions*, **2012**, 41, 8850-60	4.3	28
102	A dipole polarizable potential for reduced and doped CeO(2) obtained from first principles. *Journal of Physics Condensed Matter*, **2011**, 23, 255402	1.8	28
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100	A theoretical and experimental study of the distorted pyrochlore Bi2Sn2O7. *Journal of Materials Chemistry*, **2006**, 16, 3452		27
99	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		27
98	Lone-Pair Stabilization in Transparent Amorphous Tin Oxides: A Potential Route to p-Type Conduction Pathways. *Chemistry of Materials*, **2016**, 28, 4706-4713	9.6	26
97	Modelling inorganic solids and their interfaces: a combined approach of atomistic and electronic structure simulation techniques. *Faraday Discussions*, **2003**, 124, 155-70; discussion 205-13, 453-5	3.6	26
96	Electronic and surface properties of Ga-doped In2O3 ceramics. *Applied Surface Science*, **2015**, 349, 970-982	3.7	25
95	The nature of oxygen states on the surfaces of CeO2 and La-doped CeO2. *Chemical Physics Letters*, **2014**, 608, 239-243	2.5	25
94	Atomistic simulation of mineral surfaces: Studies of surface stability and growth. *Phase Transitions*, **1997**, 61, 83-107	1.3	25

93	On the involvement of the shallow core 5d level in the bonding in HgO. *Chemical Physics Letters*, **2004**, 399, 98-101	2.5	25
92	Valence band modification of Cr2O3 by Ni-doping: creating a high figure of merit p-type TCO. *Journal of Materials Chemistry C*, **2017**, 5, 12610-12618	7.1	24
91	The Use of the “+U” Correction in Describing Defect States at Metal Oxide Surfaces: Oxygen Vacancies on CeO2 and TiO2, and Li-doping of MgO. *E-Journal of Surface Science and Nanotechnology*, **2009**, 7, 389-394	0.7	24
90	PbO2: from semi-metal to transparent conducting oxide by defect chemistry control. *Chemical Communications*, **2013**, 49, 448-50	5.8	23
89	Energy-band alignment of II-VI/Zn3P2 heterojunctions from x-ray photoemission spectroscopy. *Journal of Applied Physics*, **2013**, 113, 203705	2.5	23
88	Comparison of the defective pyrochlore and ilmenite polymorphs of AgSbO3 using GGA and hybrid DFT. *Physical Review B*, **2011**, 83,	3.3	23
87	"Turn-on" fluorescence sensing of volatile organic compounds using a 4-amino-1,8-naphthalimide Tröger's base functionalised triazine organic polymer. *Chemical Communications*, **2019**, 55, 12140-12143	5.8	22
86	Reversible adsorption and storage of secondary explosives from water using a Tröger's base-functionalised polymer. *Journal of Materials Chemistry A*, **2017**, 5, 25014-25024	13	22
85	Chemical bonding in copper-based transparent conducting oxides: CuMO2 (M = In, Ga, Sc). *Journal of Physics Condensed Matter*, **2011**, 23, 334201	1.8	22
84	Computer aided design of nano-structured materials with tailored ionic conductivities. *Physical Chemistry Chemical Physics*, **2005**, 7, 16-8	3.6	22
83	A comparative study of the electronic structures of SrCu2O2 and PbCu2O2 by density functional theory, high resolution X-ray photoemission and electron paramagnetic resonance spectroscopy. *Journal of Materials Chemistry*, **2008**, 18, 2798		21
82	Atomistic structure of oxide nanoparticles supported on an oxide substrate. *Physical Review B*, **2002**, 65,	3.3	21
81	Atomistic simulation methodologies for modelling the nucleation, growth and structure of interfaces. *Journal of Materials Chemistry*, **2000**, 10, 1315-1324		21
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79	Molecular dynamics simulation of fluoride-perovskites. *Journal of Physics Condensed Matter*, **1992**, 4, 2097-2108	1.8	20
78	Correlating Lithium Hydroxyl Accumulation with Capacity Retention in V2O5 Aerogel Cathodes. *ACS Applied Materials & Interfaces*, **2016**, 8, 11532-8	9.5	19
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76	Band gap engineering of In2O3 by alloying with Tl2O3. *Applied Physics Letters*, **2013**, 103, 262108	3.4	18

75	Electronic energy changes associated with Guanine quadruplex formation: an investigation at the atomic level. *Journal of Physical Chemistry B*, **2010**, 114, 9833-9	3.4	18
74	Quartz amorphization: A dynamical instability. *Philosophical Magazine Letters*, **1995**, 71, 59-64	1	18
73	Modelling the electronic structure of orthorhombic LaMnO3. *Solid State Ionics*, **2017**, 299, 13-17	3.3	17
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70	Atomistic simulation of crystal growth at the a<100> screw dislocation terminating at the {100} surface of MgO. *Surface Science*, **2001**, 474, L185-L190	1.8	17
69	Assessing the potential of Mg-doped CrO as a novel p-type transparent conducting oxide. *Journal of Physics Condensed Matter*, **2016**, 28, 125501	1.8	16
68	Modelling oxygen defects in orthorhombic LaMnO and its low index surfaces. *Physical Chemistry Chemical Physics*, **2017**, 19, 24636-24646	3.6	16
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65	Simulated amorphisation and recrystallisation:nanocrystallites within meso-scale supported oxides. *Journal of Materials Chemistry*, **2000**, 10, 2241-2243		16
64	Quasiparticle Calculations on Lead-Free Hybrid Germanium Iodide Perovskite CHNHGeI for Photovoltaic Applications. *ACS Omega*, **2019**, 4, 5661-5669	3.9	15
63	Computational approach to the basicity of a series of alpha1-adrenoceptor ligands in aqueous solution. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 2850-5	3.4	15
62	Computational study of antagonist/alpha1A adrenoceptor complexes--observations of conformational variations on the formation of ligand/receptor complexes. *Journal of Medicinal Chemistry*, **2006**, 49, 501-10	8.3	15
61	Synthesis, structure and ionic conductivity in nanopolycrystalline BaF2/CaF2 heterolayers. *Chemical Communications*, **2003**, 1804-6	5.8	15
60	Dislocations, lattice slip, defects and rotated domains: The effect of a lattice misfit on supported thin-film metal oxides. *Physical Chemistry Chemical Physics*, **2000**, 2, 5491-5499	3.6	15
59	Structural exploration of thin-film oxide interfaces via simulated amorphisation and recrystallisation *Surface Science*, **2001**, 473, 97-107	1.8	15
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57	Sulfonylation of substituted benzenes using Zn-exchanged zeolites. *Journal of Molecular Catalysis A* , **2002**, 178, 205-209		14
56	Valence States in CeVO4 and Ce0.5Bi0.5VO4 Probed by Density Functional Theory Calculations and X-ray Photoemission Spectroscopy. *Journal of Physical Chemistry C*, **2014**, 118, 25330-25339	3.8	13
55	Stability, geometry, and electronic structure of an alternative I-III-VI2 material, CuScS2: A hybrid density functional theory analysis. *Applied Physics Letters*, **2010**, 97, 131904	3.4	13
54	Dehydration of butan-2-ol using modified zeolite crystals. *Applied Catalysis A: General*, **1999**, 182, 75-84	5.1	13
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49	Atomistic simulation of the effect of temperature and pressure on point defect formation in MgSiO3perovskite and the stability of CaSiO3perovskite. *Journal of Physics Condensed Matter*, **2000** , 12, 8427-8438	1.8	12
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