Nicholas Harrison

List of Publications by Year
in descending order

214 papers	12,731 citations	20797 60 h-index	27389 106 g-index
221 all docs	221 docs citations	221 times ranked	12907 citing authors

#	Article	IF	Citations
1	On the prediction of band gaps from hybrid functional theory. Chemical Physics Letters, 2001, 342, 397-401.	1.2	837
2	Electronic structure and magnetic properties of graphitic ribbons. Physical Review B, 2007, 75, .	1.1	598
3	First-principles calculations of the phase stability ofTiO2. Physical Review B, 2002, 65, .	1.1	464
4	Ab initiostudy of MnO and NiO. Physical Review B, 1994, 50, 5041-5054.	1.1	441
5	Stability of Polar Oxide Surfaces. Physical Review Letters, 2001, 86, 3811-3814.	2.9	400
6	The hardest known oxide. Nature, 2001, 410, 653-654.	13.7	316
7	Mixed Dissociative and Molecular Adsorption of Water on the Rutile (110) Surface. Physical Review Letters, 1998, 80, 762-765.	2.9	310
8	Analytical Hartree-Fock gradients for periodic systems. International Journal of Quantum Chemistry, 2001, 82, 1-13.	1.0	280
9	High-resolution DNA analysis of human embryonic stem cell lines reveals culture-induced copy number changes and loss of heterozygosity. Nature Biotechnology, 2010, 28, 371-377.	9.4	258
10	Dynamics of Single Fe Atoms in Graphene Vacancies. Nano Letters, 2013, 13, 1468-1475.	4.5	228
11	Effect of Diffusion on Lithium Intercalation in Titanium Dioxide. Physical Review Letters, 2001, 86, 1275-1278.	2.9	215
12	Structural transformations in graphene studied with high spatial and temporal resolution. Nature Nanotechnology, 2009, 4, 500-504.	15.6	203
13	First-principles spin-polarized calculations on the reduced and reconstructedTiO2(110) surface. Physical Review B, 1997, 55, 15919-15927.	1.1	191
14	Water chemistry on surface defect sites: Chemidissociation versus physisorption on MgO(001). Journal of Chemical Physics, 1994, 101, 1547-1554.	1.2	189
15	Spin Singlet Formation inMgTi2O4: Evidence of a Helical Dimerization Pattern. Physical Review Letters, 2004, 92, 056402.	2.9	178
16	First-principles molecular dynamics simulation of water dissociation on TiO2 (110). Chemical Physics Letters, 1996, 261, 246-252.	1.2	160
17	Revisiting the Surface Structure ofTiO2(110): A Quantitative low-Energy Electron Diffraction Study. Physical Review Letters, 2005, 94, .	2.9	154
18	The group IIIâ€“V's semiconductor energy gaps predicted using the B3LYP hybrid functional. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 2125-2127.	1.3	146

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19	An ab initio study of ZnO(101Ì„0). Surface Science, 2000, 457, L342-L346.	0.8	136
20	Absorption characteristics of a quantum dot array induced intermediate band: Implications for solar cell design. Applied Physics Letters, 2008, 93, 263105.	1.5	135
21	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	1.2	133
22	Lattice dynamics of TiO2 rutile: influence of gradient corrections in density functional calculations. Chemical Physics Letters, 2002, 364, 528-534.	1.2	132
23	Structural Reconstruction of the Graphene Monovacancy. ACS Nano, 2013, 7, 4495-4502.	7.3	131
24	A defective graphene phase predicted to be a room temperature ferromagnetic semiconductor. New Journal of Physics, 2008, 10, 033002.	1.2	130
25	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
26	Chlorine adsorption on the Cu(111) surface. Chemical Physics Letters, 2000, 317, 282-289.	1.2	120
27	Stability of rocksalt polar surfaces:â€‚â€‚Anab initiostudy of MgO(111) and NiO(111). Physical Review B, 2003, 68, .	1.1	116
28	Electronic and magnetic structure ofLaMnO3from hybrid periodic density-functional theory. Physical Review B, 2004, 69, .	1.1	116
29	Diffusion of Li-ions in rutile. An ab initio study. Solid State Ionics, 2003, 157, 35-38.	1.3	113
30	Density-functional simulations of lithium intercalation in rutile. Physical Review B, 2002, 65, .	1.1	110
31	The influence of soft vibrational modes on our understanding of oxide surface structure. Faraday Discussions, 1999, 114, 305-312.	1.6	106
32	Ab initio study of high pressure phase transition in GaN. Journal of Physics and Chemistry of Solids, 1994, 55, 1357-1361.	1.9	99
33	Comment on â€œAbout the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction errorâ€•[J. Chem. Phys. 123, 164110 (2005)]. Journal of Chemical Physics, 2006, 124, 107101.	1.2	99
34	The stability of polar oxide surfaces: The interaction of H2O with ZnO(0001) and ZnO(0001Ì„). Journal of Chemical Physics, 2001, 115, 2312-2316.	1.2	98
35	Structure and properties of ilmenite from first principles. Physical Review B, 2005, 71, .	1.1	98
36	Ab initiodetermination of the bulk properties of MgO. Physical Review B, 1994, 49, 8574-8582.	1.1	96

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37	Anab initio Hartreeâ€“Fock study of Î±-MoO3. Journal of Materials Chemistry, 1997, 7, 959-967.	6.7	96
38	Ab initioHartree-Fock calculations of CaO, VO, MnO and NiO. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1993, 68, 653-666.	0.7	95
39	Influence of water intercalation and hydration on chemical decomposition and ion transport in methylammonium lead halide perovskites. Journal of Materials Chemistry A, 2018, 6, 1067-1074.	5.2	94
40	Ab initio study of ZnO (101Â¯0) surface relaxation. Physical Review B, 1994, 49, 11153-11158.	1.1	92
41	Thermodynamics of oxygen defective MagnÃ©li phases in rutile: A first-principles study. Physical Review B, 2008, 77, .	1.1	92
42	Magnetic coupling constants from a hybrid density functional with 35% Hartree-Fock exchange. Physical Review B, 2004, 70, .	1.1	91
43	An ab-initio study of ZnO(112Ì„0). Surface Science, 2000, 468, L851-L855.	0.8	86
44	Effects of exchange, correlation, and numerical approximations on the computed properties of the rutileTiO2(100) surface. Physical Review B, 1999, 59, 2320-2326.	1.1	84
45	Structure of the Î±-Cr2O3(0001) surface: Anab initiototal-energy study. Physical Review B, 1996, 54, 14066-14070.	1.1	80
46	Electronic structure of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ti</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub phase. Physical Review B, 2009, 79, .	1.1	78
47	High-temperature antiferromagnetism in molecular semiconductor thin films and nanostructures. Nature Communications, 2014, 5, 3079.	5.8	76
48	An ab initio Hartree-Fock study of the electron-excess gap states in oxygen-deficient rutile TiO2. Surface Science, 1997, 384, 192-200.	0.8	74
49	A density functional study of lithium bulk and surfaces. Journal of Physics Condensed Matter, 1999, 11, 5007-5019.	0.7	74
50	Magnetic properties of polymerizedC60: The influence of defects and hydrogen. Physical Review B, 2004, 70, .	1.1	71
51	Orthorhombic distortion on Li intercalation in anatase. Physical Review B, 2004, 69, .	1.1	71
52	Simulation of low index rutile surfaces with a transferable variable-charge Tiâ€“O interatomic potential and comparison with ab initio results. Surface Science, 2002, 504, 115-124.	0.8	70
53	On-site interband excitations in resonant inelastic x-ray scattering from<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math>. Physical Review B, 2008, 77, .	1.1	70
54	Ab initio simulation of molecular processes on oxide surfaces. Faraday Discussions, 1997, 106, 135-154.	1.6	69

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55	Investigation of the Switching Mechanism in TiO₂-Based RRAM: A Two-Dimensional EDX Approach. ACS Applied Materials & Interfaces, 2016, 8, 19605-19611.	4.0	69
56	An experimental and theoretical investigation of the electronic structure of CdO. Journal of Physics Condensed Matter, 1998, 10, 8447-8458.	0.7	68
57	Comparison of a combined quantum mechanics/interatomic potential function approach with its periodic quantum-mechanical limit: Proton siting and ammonia adsorption in zeolite chabazite. Journal of Chemical Physics, 1998, 109, 10379-10389.	1.2	66
58	Open circuit voltage profile for Li-intercalation in rutile and anatase from first principles. Solid State Ionics, 2002, 152-153, 189-194.	1.3	65
59	Vibrational Analysis Study of Aluminum Trifluoride Phases. Journal of Physical Chemistry A, 2007, 111, 5813-5819.	1.1	63
60	Defect physics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CuGaS</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2010, 81, .	1.1	62
61	Metal-insulator and magnetic transition of NiO at high pressures. Physical Review B, 2004, 69, .	1.1	60
62	First-principles study of potassium adsorption onTiO2surfaces. Physical Review B, 1999, 59, 15457-15463.	1.1	59
63	Linear-scaling time-dependent density-functional theory in the linear response formalism. Journal of Chemical Physics, 2013, 139, 064104.	1.2	59
64	Theoretical study of chlorine adsorption on the Ag(111) surface. Physical Review B, 2001, 63, .	1.1	57
65	Direct evidence of O(p) holes in Li-doped NiO from Hartree-Fock calculations. Chemical Physics Letters, 1996, 250, 66-70.	1.2	56
66	The structural relaxation of the Î±-Al2O3(0001) â€“ an investigation of potential errors. Chemical Physics Letters, 2001, 341, 412-418.	1.2	54
67	The TiO2(100)(1 Ã— 3) reconstruction: insights from ab initio calculations. Surface Science, 1996, 364, 431-438.	0.8	52
68	An ab initio study of Î±-Al2O3(0001): the effects of exchange and correlation functionals. Surface Science, 2000, 458, 25-33.	0.8	52
69	First-principles study of H intercalation in rutileTiO2. Physical Review B, 2004, 70, .	1.1	52
70	Surface model and exchange-correlation functional effects on the description of Pd/Î±-Al2O3(0001). Journal of Chemical Physics, 2002, 116, 1684-1691.	1.2	51
71	First-principles optical response of semiconductors and oxide materials. Physical Review B, 2011, 83, .	1.1	51
72	An ab initio study of oxygen adsorption on tin dioxide. Surface Science, 2008, 602, 1072-1079.	0.8	49

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73	Electronic and Optical Structure of Wurtzite CuInS₂. Journal of Physical Chemistry C, 2014, 118, 14478-14484.	1.5	49
74	Dynamics of Paramagnetic Metallofullerenes in Carbon Nanotube Peapods. Nano Letters, 2008, 8, 1005-1010.	4.5	48
75	Electronic structure of Lewis acid sites on high surface area aluminium fluorides: a combined XPS and ab initio investigation. Physical Chemistry Chemical Physics, 2009, 11, 5664.	1.3	48
76	Structure and Stability of Î±-AlF₃ Surfaces. Journal of Physical Chemistry C, 2009, 113, 4976-4983.	1.5	48
77	An efficient method for computing the binding energy of an adsorbed molecule within a periodic approach. The application to vinyl fluoride at rutile TiO2(1 1 0) surface. Computational Materials Science, 2011, 50, 2080-2086.	1.4	48
78	The high-pressure phase transitions of silicon and gallium nitride: a comparative study of Hartree - Fock and density functional calculations. Journal of Physics Condensed Matter, 1996, 8, 3993-4000.	0.7	43
79	An ab Initio Study of Hydrogen Adsorption on ZnO(101Ì„0). Journal of Physical Chemistry B, 2001, 105, 6191-6193.	1.2	43
80	Aluminum Chloride as a Solid Is Not a Strong Lewis Acid. Journal of Physical Chemistry B, 2006, 110, 8314-8319.	1.2	43
81	A quantum-mechanical study of the vinyl fluoride adsorbed on the rutile TiO2(110) surface. Surface Science, 2006, 600, 305-317.	0.8	43
82	First principles predictions for intercalation behaviour. Solid State Ionics, 2004, 175, 829-834.	1.3	42
83	Pressure-induced instabilities in bulk TiO2rutile. Journal of Physics Condensed Matter, 2004, 16, 273-292.	0.7	42
84	The physical and electronic structure of the rutile (001) surface. Surface Science, 2000, 446, 119-127.	0.8	41
85	Electronic structure ofCaCuO2from the B3LYP hybrid density functional. Physical Review B, 2004, 69, .	1.1	39
86	Thermodynamic stability of LaMnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>and its competing oxides: A hybrid density functional study of an alkaline fuel cell catalyst. Physical Review B, 2011, 84, .	1.1	39
87	Molecular dynamics study of TiO2 microclusters. Journal of Materials Chemistry, 1996, 6, 1385.	6.7	38
88	An ab initio Hartree-Fock investigation of galena (PbS). Chemical Physics Letters, 1996, 257, 627-632.	1.2	38
89	High-pressure phases ofFeTiO3from first principles. Physical Review B, 2005, 72, .	1.1	38
90	Magnetic moment and coupling mechanism of iron-doped rutileTiO2from first principles. Physical Review B, 2007, 75, .	1.1	38

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91	Electrochemical Characterization and Quantified Surface Termination Obtained by Low Energy Ion Scattering and X-ray Photoelectron Spectroscopy of Orthorhombic and Rhombohedral LaMnO₃ Powders. Journal of Physical Chemistry C, 2015, 119, 12209-12217.	1.5	38
92	Ab initiostudy of the surface and interfacial properties of a layered MgO/NiO film. Physical Review B, 1995, 52, 5375-5384.	1.1	35
93	Parallel implementation of the ab initio CRYSTAL program: electronic structure calculations for periodic systems. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2011, 467, 2112-2126.	1.0	35
94	Chemistry of defect induced photoluminescence in chalcopyrites: The case of CuAlS2. Journal of Applied Physics, 2011, 109, .	1.1	35
95	The structural properties of beta -MgCl2; an ab initio study. Journal of Physics Condensed Matter, 1992, 4, 3873-3882.	0.7	34
96	Density functional study of the magnetic coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>V</mml:mtext><mml:msub><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow> Physical Review B, 2009, 79, .	1.1	34
97	Geometric structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn> Confirming experimental conclusions. Physical Review B, 2010, 81, .	1.1	34
98	Periodic quantum mechanical simulation of the Heâ€“MgO(100) interaction potential. Journal of Chemical Physics, 2011, 134, 014706.	1.2	34
99	Ab initiocomplex band structure of conjugated polymers: Effects of hydrid density functional theory and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="italic">GW</mml:mi></mml:mrow></mml:math>schemes. Physical Review B, 2012, 85, .	1.1	34
100	Temporal evolution of sweet oilfield corrosion scale: Phases, morphologies, habits, and protection. Corrosion Science, 2018, 142, 110-118.	3.0	33
101	Electronic structure and exchange interactions in cobalt-phthalocyanine chains. Physical Review B, 2013, 88, .	1.1	31
102	A new phase of lithiated titania predicted from first principles. Chemical Physics Letters, 2003, 371, 150-156.	1.2	30
103	Identification of possible Lewis acid sites on the Î²-AlF3(100) surface: an ab initio total energy study. Physical Chemistry Chemical Physics, 2005, 7, 3989.	1.3	30
104	A density functional study of water and methanol chemisorption on MgO(110). Surface Science, 2005, 591, 13-22.	0.8	29
105	Water adsorption on rutile TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>(110) for applications in solar hydrogen production: A systematic hybrid-exchange density functional study. Physical Review B, 2012, 86, .	1.1	29
106	Electronic structures and phonon free energies of LaCoO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>using hybrid-exchange density functional theory. Physical Review B, 2013, 87, .	1.1	28
107	Ab initio studies of aluminium fluoride surfaces. Journal of Materials Chemistry, 2006, 16, 1906.	6.7	27
108	Stability of the AlF3 surface in H2O and HF environments: An investigation using hybrid density functional theory and atomistic thermodynamics. Surface Science, 2007, 601, 4433-4437.	0.8	27

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109	Modeling spin interactions in carbon peapods using a hybrid density functional theory. Physical Review B, 2008, 77, .	1.1	27
110	Effect of the surface model on the theoretical description of the chemisorption of atomic hydrogen on Cu(). Surface Science, 2003, 522, 185-197.	0.8	26
111	The Unusual Redox Properties of Fluoroferrocenes Revealed through a Comprehensive Study of the Haloferrocenes. Organometallics, 2015, 34, 5461-5469.	1.1	26
112	Unravelling Some of the Structureâ€“Property Relationships in Graphene Oxide at Low Degree of Oxidation. Journal of Physical Chemistry Letters, 2018, 9, 1746-1749.	2.1	26
113	A study of the energetics of the Cl2/MgO(001) interface using correlation corrected periodic Hartreeâ€“Fock theory. Journal of Chemical Physics, 1993, 98, 6387-6391.	1.2	25
114	Theoretical analysis of strain and strain decay in InAsâˆ•GaAs(001) multilayer quantum dot growth. Journal of Applied Physics, 2006, 99, 093522.	1.1	25
115	Li sites and phase stability in TiO2-anatase and Zr-doped TiO2-anatase. Journal of Materials Chemistry, 2006, 16, 1973.	6.7	25
116	The stability of LaMnO3 surfaces: a hybrid exchange density functional theory study of an alkaline fuel cell catalyst. Journal of Materials Chemistry A, 2013, 1, 11152.	5.2	25
117	First-Principles Study of the Water Adsorption on Anatase(101) as a Function of the Coverage. Journal of Physical Chemistry C, 2018, 122, 20736-20744.	1.5	25
118	Corrosion Protection through Naturally Occurring Films: New Insights from Iron Carbonate. ACS Applied Materials & Interfaces, 2019, 11, 33435-33441.	4.0	25
119	The structure of the reduced rutile TiO2(100) 1Ã—3 reconstruction. Surface Science, 2001, 479, L375-L381.	0.8	24
120	Tunable, Low Optical Loss Strontium Molybdate Thin Films for Plasmonic Applications. Advanced Optical Materials, 2017, 5, 1700622.	3.6	24
121	AbÂinitio Total Energy Studies of the Î±-Cr2O3 (0001) and $(01ar{1}2)$ Surfaces. Surface Review and Letters, 1998, 05, 337-340.	0.5	23
122	Composition and Structure of the Î±-AlF3(0001) Surface. Journal of Physical Chemistry B, 2005, 109, 22935-22938.	1.2	23
123	A quantum mechanical study of water adsorption on the (110) surfaces of rutile SnO2 and TiO2: investigating the effects of intermolecular interactions using hybrid-exchange density functional theory. Physical Chemistry Chemical Physics, 2014, 16, 21002-21015.	1.3	23
124	Structural deformations in lithium doped titanium dioxide. Computational Materials Science, 2002, 24, 235-240.	1.4	22
125	Surface to bulk charge transfer at an alkali metal/metal oxide interface. Surface Science, 2003, 547, L859-L864.	0.8	22
126	Theoretical modeling of the electronic structure and exchange interactions in a Cu(II)Pc one-dimensional chain. Physical Review B, 2011, 84, .	1.1	22

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127	A quantum-mechanical study of the adsorption of prototype dye molecules on rutile-TiO₂(110): a comparison between catechol and isonicotinic acid. Physical Chemistry Chemical Physics, 2013, 15, 235-243.	1.3	21
128	Growth of Epitaxial Oxide Thin Films on Graphene. Scientific Reports, 2016, 6, 31511.	1.6	20
129	Characterising MgF2 surfaces with CO adsorption calculations. Surface Science, 2013, 609, 73-77.	0.8	19
130	Photoemission simulation for photocathode design: theory and application to copper and silver surfaces. Computational Materials Science, 2016, 122, 331-340.	1.4	19
131	The Effect of Surface Reconstruction on the Oxygen Reduction Reaction Properties of LaMnO₃. Journal of Physical Chemistry C, 2019, 123, 11621-11627.	1.5	19
132	The Derivation of Shell Model Potentials for MgCl₂FromAb InitioTheory. Molecular Simulation, 1992, 9, 171-174.	0.9	18
133	Strain Engineering of Adsorbate Self-Assembly on Graphene for Band Gap Tuning. Journal of Physical Chemistry C, 2019, 123, 4475-4482.	1.5	18
134	An ab initio study of the magnetic coupling in bi-metallic CrIII cyanides. Chemical Physics Letters, 1997, 266, 507-511.	1.2	17
135	Effects of Doping on Electronic Structure and Correlations in Carbon Peapods. ACS Nano, 2009, 3, 1069-1076.	7.3	17
136	Electronic structure of IIIâ€“Vâ€™s semiconductors from B3LYP and PBE0 functionals. AIP Conference Proceedings, 2010, , .	0.3	17
137	Magnetic properties of copper hexadecaphthalocyanine (F16CuPc) thin films and powders. Journal of Applied Physics, 2013, 113, 013914.	1.1	17
138	Approaching an exact treatment of electronic correlations at solid surfaces: The binding energy of the lowest bound state of helium adsorbed on MgO(100). Physical Review B, 2014, 89, .	1.1	17
139	Beyond band bending in the WO₃/BiVO₄ heterojunction: insight from DFT and experiment. Sustainable Energy and Fuels, 2019, 3, 264-271.	2.5	17
140	Molecular dynamics study of the high temperature fusion of TiO2 nanoclusters. Journal of Materials Chemistry, 1997, 7, 2543-2546.	6.7	16
141	The structure of higher defective ZnO (101Ì„0). Surface Science, 2003, 529, L281-L284.	0.8	16
142	Half-metallicity in the ferrimagnet<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Nb</mml:mtext><mml:msub><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow	1.1	16
	first principles. Physical Review B, 2010, 82, .		
143	Chemical Descriptors of Yttria-Stabilized Zirconia at Low Defect Concentration: An ab Initio Study. Journal of Physical Chemistry A, 2015, 119, 6412-6420.	1.1	16
144	Optimizing Oxygen Reduction Catalyst Morphologies from First Principles. Journal of Physical Chemistry C, 2015, 119, 16804-16810.	1.5	16

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145	Transition metal materials: a first principles approach to the electronic structure of the insulating phase. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 1998, 356, 75-88.	1.6	15
146	Hybrid exchange density functional study of vicinal anatase<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>surfaces. Physical Review B, 2014, 89, .	1.1	15
147	The atomistic structure of yttria stabilised zirconia at 6.7 mol%: an ab initio study. Physical Chemistry Chemical Physics, 2016, 18, 31277-31285.	1.3	15
148	Adsorption of HF and HCl on the Î²-AlF3 (100) surface. Physical Chemistry Chemical Physics, 2008, 10, 2918.	1.3	14
149	Steps, Microfacets, and Crystal Morphology:â€‰ An ab Initio Study of Î²-AlF₃Surfaces. Journal of Physical Chemistry C, 2008, 112, 6515-6519.	1.5	14
150	Optical properties of alkali halide crystals from all-electron hybrid TD-DFT calculations. Journal of Chemical Physics, 2015, 142, 214705.	1.2	14
151	Localized electron behaviour within band theory a Hartree-Fock description of MxMg1-xO(M=Mn, Ni). Journal of Physics Condensed Matter, 1995, 7, 6231-6239.	0.7	13
152	Hybrid density functional study of structural, bonding, and electronic properties of the manganite series<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">La</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mtext>â^’</mml:mtext><mml:mi>x</mml:mi></mml:mro xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Ca</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:math><mml:math xmlns:mml="http://www.w3.org/1998/Math/M. Physical Review B, 2014, 89, .	1.1	13
153	Correlation functional estimates of the dispersion intraction in semi-ionic compounds. Journal of Physics Condensed Matter, 1992, 4, L261-L264.	0.7	12
154	Optical response of extended systems from time-dependent Hartree-Fock and time-dependent density-functional theory. Journal of Physics: Conference Series, 2012, 367, 012001.	0.3	12
155	Ab initiotheory of magnetic interactions at surfaces. Journal of Physics Condensed Matter, 2004, 16, S2557-S2574.	0.7	11
156	Hybrid density functional study of organic magnetic crystals: bi-metallic CrIIIcyanides and rhombohedral C60. Molecular Physics, 2005, 103, 2573-2585.	0.8	11
157	He-atom scattering from MgO(100): calculating diffraction peak intensities with a semi ab initio potential. Physical Chemistry Chemical Physics, 2011, 13, 14750.	1.3	11
158	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-orbital nanomagnetism in an organic chain magnet. Physical Review B, 2013, 88, .	1.1	11
159	Diffraction of helium on MgO(100) surface calculated from first-principles. Physical Chemistry Chemical Physics, 2014, 16, 21106-21113.	1.3	11
160	Density functional study of the electronic and vibrational properties of TiOCl. Physical Review B, 2007, 76, .	1.1	10
161	Characterization of Lewis acid sites on the (100) surface of Î²-AlF3: Ab initio calculations of NH3 adsorption. Journal of Chemical Physics, 2008, 128, 224703.	1.2	10
162	Reactivity of the Î²-AlF3(100) surface: defects, fluorine mobility and catalysis of the CCl2F2 dismutation reaction. Physical Chemistry Chemical Physics, 2010, 12, 6124.	1.3	10

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