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	Corrosion inhibition in acidic environments: key interfacial insights with photoelectron spectroscopy. Faraday Discussions, 2022, 236, 374-388.	1.6	6
2	Monomolecular Cracking of Propane: Effect of Zeolite Confinement and Acidity. ACS Omega, 2022, 7, 7531-7540.	1.6	7
3	A transferable prediction model of molecular adsorption on metals based on adsorbate and substrate properties. Physical Chemistry Chemical Physics, 2022, 24, 16545-16555.	1.3	3
4	Diffusivity of Propylene in One-Dimensional Medium-Pore Zeolites. Journal of Physical Chemistry C, 2021, 125, 19200-19208.	1.5	8
5	Properties and degradation of manganese(III) porphyrin thin films formed by high vacuum sublimation. , 2021, , 924-931.		0
6	Ripples in isotropically compressed graphene. Computational Materials Science, 2020, 173, 109422.	1.4	6
7	The CRYSTAL code, 1976â€“2020 and beyond, a long story. Journal of Chemical Physics, 2020, 152, 204111.	1.2	133
8	Core level photoemission line shape selection: Atomic adsorbates on iron. Surface and Interface Analysis, 2020, 52, 507-512.	0.8	6
9	Theoretical study of the influence of hydrides on the performance of Mg and Y photocathodes. Journal of Applied Physics, 2020, 127, 025304.	1.1	0
10	From Electronic Structure to Design Principles for Photocathodes: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Cu</mml:mi></mml:math> - <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mi>Ba</mml:mi></mml:math> Alloys. Physical Review Applied, 2019, 11, .	1.5	2
11	Corrosion Protection through Naturally Occurring Films: New Insights from Iron Carbonate. ACS Applied Materials & Interfaces, 2019, 11, 33435-33441.	4.0	25
12	Beyond band bending in the WO₃/BiVO₄ heterojunction: insight from DFT and experiment. Sustainable Energy and Fuels, 2019, 3, 264-271.	2.5	17
13	Strain Engineering of Adsorbate Self-Assembly on Graphene for Band Gap Tuning. Journal of Physical Chemistry C, 2019, 123, 4475-4482.	1.5	18
14	First Principles Calculations on the Stoichiometric and Defective (101) Anatase Surface and Upon Hydrogen and H2Pc Adsorption: The Influence of Electronic Exchange and Correlation and of Basis Set Approximations. Frontiers in Chemistry, 2019, 7, 220.	1.8	6
15	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
16	Properties and degradation of manganese(III) porphyrin thin films formed by high vacuum sublimation. Journal of Porphyrins and Phthalocyanines, 2019, 23, 1515-1522.	0.4	2
17	Work function and quantum efficiency study of metal oxide thin films on Ag(100). Physical Review B, 2018, 97, .	1.1	7
18	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

#	Article	IF	Citations
19	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
20	Temporal evolution of sweet oilfield corrosion scale: Phases, morphologies, habits, and protection. Corrosion Science, 2018, 142, 110-118.	3.0	33
21	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
22	A model for time-dependent grain boundary diffusion of ions and electrons through a film or scale, with an application to alumina. Acta Materialia, 2017, 132, 503-516.	3.8	3
23	Tunable, Low Optical Loss Strontium Molybdate Thin Films for Plasmonic Applications. Advanced Optical Materials, 2017, 5, 1700622.	3.6	24
24	A hybrid-exchange density functional study of the bonding and electronic structure in bulk CuFeS2. Journal of Chemical Physics, 2016, 144, 184702.	1.2	9
25	Photoemission simulation for photocathode design: theory and application to copper and silver surfaces. Computational Materials Science, 2016, 122, 331-340.	1.4	19
26	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
27	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
28	Growth of Epitaxial Oxide Thin Films on Graphene. Scientific Reports, 2016, 6, 31511.	1.6	20
29	A combined thermodynamics and first principles study of the electronic, lattice and magnetic contributions to the magnetocaloric effect in La0.75Ca0.25MnO3. Journal Physics D: Applied Physics, 2016, 49, 285001.	1.3	3
30	Structure of a Model Dye/Titania Interface: Geometry of Benzoate on Rutile-TiO₂ (110)(1 Ã—) Tj ETQq0 0 0 rgBT /Overlock	1.5	6
31	Surface morphology ofCuFeS2: The stability of the polar(112)/(112Â¯)surface pair. Physical Review B, 2015, 92, .	1.1	10
32	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
33	Thin film properties of tetracyanoquinodimethane (TCNQ) with novel templating effects. Journal of Materials Chemistry C, 2015, 3, 8694-8699.	2.7	8
34	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
35	Optimizing Oxygen Reduction Catalyst Morphologies from First Principles. Journal of Physical Chemistry C, 2015, 119, 16804-16810.	1.5	16
36	The Unusual Redox Properties of Fluoroferrocenes Revealed through a Comprehensive Study of the Haloferrocenes. Organometallics, 2015, 34, 5461-5469.	1.1	26

#	Article	IF	Citations
37	Optical properties of alkali halide crystals from all-electron hybrid TD-DFT calculations. Journal of Chemical Physics, 2015, 142, 214705.	1.2	14
38	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
39	High-temperature antiferromagnetism in molecular semiconductor thin films and nanostructures. Nature Communications, 2014, 5, 3079.	5.8	76
40	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
41	Diffraction of helium on MgO(100) surface calculated from first-principles. Physical Chemistry Chemical Physics, 2014, 16, 21106-21113.	1.3	11
42	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
43	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
44	Electronic and Optical Structure of Wurtzite CuInS₂. Journal of Physical Chemistry C, 2014, 118, 14478-14484.	1.5	49
45	A hybrid-exchange density functional study of Ca-doped LaMnO3. Journal of Applied Physics, 2013, 113, 17A910.	1.1	9
46	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
47	Linear-scaling time-dependent density-functional theory in the linear response formalism. Journal of Chemical Physics, 2013, 139, 064104.	1.2	59
48	<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
49	Determining Surface Chemistry and Vibrational Properties of SOFC Anode Materials Through Ab Initio Calculations. ECS Transactions, 2013, 57, 2419-2427.	0.3	2
50	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
51	Characterising MgF2 surfaces with CO adsorption calculations. Surface Science, 2013, 609, 73-77.	0.8	19
52	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
53	Dynamics of Single Fe Atoms in Graphene Vacancies. Nano Letters, 2013, 13, 1468-1475.	4.5	228
54	Structural Reconstruction of the Graphene Monovacancy. ACS Nano, 2013, 7, 4495-4502.	7.3	131

#	Article	IF	Citations
55	The structure of water on rutile TiO2(110) for applications in solar hydrogen production: towards a predictive model using hybrid-exchange density functional theory. Materials Research Society Symposia Proceedings, 2013, 1542, 1.	0.1	0
56	Simulating Constant Current STM Images of the Rutile TiO₂ (110) Surface for Applications in Solar Water Splitting. Materials Research Society Symposia Proceedings, 2013, 1494, 339-344.	0.1	3
57	Magnetic properties of copper hexadecaphthalocyanine (F16CuPc) thin films and powders. Journal of Applied Physics, 2013, 113, 013914.	1.1	17
58	Electronic structure and exchange interactions in cobalt-phthalocyanine chains. Physical Review B, 2013, 88, .	1.1	31
59	Comment on â€œFirst-principles study of the influence of (110)-oriented strain on the ferroelectric properties of 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>â€• Physical Review B, 2013, 88, .	1.1	9
60	Suitability of chromium phthalocyanines to test Haldane's conjecture: First-principles calculations. Physical Review B, 2013, 88, .	1.1	8
61	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
62	Comment on â€œ2D Atomic Mapping of Oxidation States in Transition Metal Oxides by Scanning Transmission Electron Microscopy and Electron Energy-Loss Spectroscopyâ€• Physical Review Letters, 2012, 108, 259701; discussion 259702.	2.9	9
63	Theoretical modeling of the electronic structure and exchange interactions in Cu(II)Pc. Journal of Physics: Conference Series, 2012, 391, 012119.	0.3	1
64	Atomic structure of the (001) surface of CuGaSe2. Surface Science, 2012, 606, 496-504.	0.8	4
65	Influence of background carriers on magnetic properties of Mn-doped dilute magnetic Si. Journal of Magnetism and Magnetic Materials, 2012, 324, 3748-3753.	1.0	4
66	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
67	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
68	Ab initio calculation of the MgO(100) interaction with He and Ne: a HF + MP2 and HF + MP2(B3LYP) comparison. Chemical Communications, 2011, 47, 11630.	2.2	2
69	An alternative approach for the calculation of correlation energy in periodic systems: a hybrid MP2(B3LYP) study of the Heâ€“MgO(100) interaction. Chemical Communications, 2011, 47, 4385.	2.2	7
70	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
71	First-principles optical response of semiconductors and oxide materials. Physical Review B, 2011, 83, .	1.1	51
72	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

#	Article	IF	Citations
73	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
74	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
75	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
76	Chemistry of defect induced photoluminescence in chalcopyrites: The case of CuAlS2. Journal of Applied Physics, 2011, 109, .	1.1	35
77	Periodic quantum mechanical simulation of the Heâ€“MgO(100) interaction potential. Journal of Chemical Physics, 2011, 134, 014706.	1.2	34
78	Calculating charged defects using CRYSTAL. Journal of Physics: Conference Series, 2010, 242, 012004.	0.3	6
79	Electronic structure of IIIâ€“Vâ€™s semiconductors from B3LYP and PBE0 functionals. AIP Conference Proceedings, 2010, , .	0.3	17
80	Absorption characteristics of intermediate band solar cell. , 2010, , .		3
81	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
82	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 first principles. Physical Review B, 2010, 82, .	1.1	16
83	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
84	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> Physical Review B, 2010, 81, .	1.1	62
85	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
86	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
87	Stability of the ferromagnetic state in a mixed<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>2</mml:mn></mml:msup> system. Physical Review B, 2009, 80, .	1.1	6
88	Structural transformations in graphene studied with high spatial and temporal resolution. Nature Nanotechnology, 2009, 4, 500-504.	15.6	203
89	Effects of Doping on Electronic Structure and Correlations in Carbon Peapods. ACS Nano, 2009, 3, 1069-1076.	7.3	17
90	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

#	Article	IF	Citations
91	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
92	Structure and Stability of Î±-AlF₃ Surfaces. Journal of Physical Chemistry C, 2009, 113, 4976-4983.	1.5	48
93	Electronic structure of QD arrays: application to intermediate-band solar cells. Optical and Quantum Electronics, 2008, 40, 313-318.	1.5	8
94	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
95	An ab initio study of oxygen adsorption on tin dioxide. Surface Science, 2008, 602, 1072-1079.	0.8	49
96	Modeling spin interactions in carbon peapods using a hybrid density functional theory. Physical Review B, 2008, 77, .	1.1	27
97	A defective graphene phase predicted to be a room temperature ferromagnetic semiconductor. New Journal of Physics, 2008, 10, 033002.	1.2	130
98	Dynamics of Paramagnetic Metallofullerenes in Carbon Nanotube Peapods. Nano Letters, 2008, 8, 1005-1010.	4.5	48
99	Adsorption of HF and HCl on the Î²-AlF3 (100) surface. Physical Chemistry Chemical Physics, 2008, 10, 2918.	1.3	14
100	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
101	Absorption characteristics of a quantum dot array induced intermediate band: Implications for solar cell design. Applied Physics Letters, 2008, 93, 263105.	1.5	135
102	Thermodynamics of oxygen defective MagnÃ©li phases in rutile: A first-principles study. Physical Review B, 2008, 77, .	1.1	92
103	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
104	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
105	First principles characterisation of aluminium trifluoride catalysts. Journal of Physics: Conference Series, 2008, 117, 012004.	0.3	7
106	Investigating the Lewis acidity of aluminium fluoride surfaces. Journal of Physics: Conference Series, 2008, 100, 012009.	0.3	0
107	Magnetic moment and coupling mechanism of iron-doped rutileTiO2from first principles. Physical Review B, 2007, 75, .	1.1	38
108	Density functional study of the electronic and vibrational properties of TiOCl. Physical Review B, 2007, 76, .	1.1	10

#	Article	IF	Citations
109	Analysis of Strain-Decay in InAs/GaAs(001) Multilayer Quantum Dot Growth. AIP Conference Proceedings, 2007, , .	0.3	0
110	Electronic structure of QD arrays: Application to intermediate-band solar cells. , 2007, , .		0
111	Vibrational Analysis Study of Aluminum Trifluoride Phases. Journal of Physical Chemistry A, 2007, 111, 5813-5819.	1.1	63
112	Electronic structure and magnetic properties of graphitic ribbons. Physical Review B, 2007, 75, .	1.1	598
113	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
114	The electronic structure of SrCu2O2 studied by synchrotron radiation excited photoemission and hybrid exchange density functional calculations. Chemical Physics Letters, 2007, 450, 39-43.	1.2	6
115	Ab initio studies of aluminium fluoride surfaces. Journal of Materials Chemistry, 2006, 16, 1906.	6.7	27
116	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
117	Li sites and phase stability in TiO2-anatase and Zr-doped TiO2-anatase. Journal of Materials Chemistry, 2006, 16, 1973.	6.7	25
118	Aluminum Chloride as a Solid Is Not a Strong Lewis Acid. Journal of Physical Chemistry B, 2006, 110, 8314-8319.	1.2	43
119	Ferromagnetism in Defective Polymerised C 60. , 2006, , 523-540.		0
120	A quantum-mechanical study of the vinyl fluoride adsorbed on the rutile TiO2(110) surface. Surface Science, 2006, 600, 305-317.	0.8	43
121	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
122	A density functional study of water and methanol chemisorption on MgO(110). Surface Science, 2005, 591, 13-22.	0.8	29
123	Revisiting the Surface Structure ofTiO2(110): A Quantitative low-Energy Electron Diffraction Study. Physical Review Letters, 2005, 94, .	2.9	154
124	High-pressure phases ofFeTiO3from first principles. Physical Review B, 2005, 72, .	1.1	38
125	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
126	Composition and Structure of the Î±-AlF3(0001) Surface. Journal of Physical Chemistry B, 2005, 109, 22935-22938.	1.2	23

#	Article	IF	Citations
127	Hybrid density functional study of organic magnetic crystals: bi-metallic CrIIIcyanides and rhombohedral C60. Molecular Physics, 2005, 103, 2573-2585.	0.8	11
128	Structure and properties of ilmenite from first principles. Physical Review B, 2005, 71, .	1.1	98
129	Ab initiotheory of magnetic interactions at surfaces. Journal of Physics Condensed Matter, 2004, 16, S2557-S2574.	0.7	11
130	Magnetic coupling constants from a hybrid density functional with 35% Hartree-Fock exchange. Physical Review B, 2004, 70, .	1.1	91
131	First-principles study of H intercalation in rutileTiO2. Physical Review B, 2004, 70, .	1.1	52
132	Magnetic properties of polymerizedC60: The influence of defects and hydrogen. Physical Review B, 2004, 70, .	1.1	71
133	Spin Singlet Formation inMgTi2O4: Evidence of a Helical Dimerization Pattern. Physical Review Letters, 2004, 92, 056402.	2.9	178
134	Electronic structure ofCaCuO2from the B3LYP hybrid density functional. Physical Review B, 2004, 69, .	1.1	39
135	Hydrogen Intercalation Sites in Rutile Predicted from Ab Initio Calculations. Materials Research Society Symposia Proceedings, 2004, 813, 341.	0.1	0
136	First principles predictions for intercalation behaviour. Solid State Ionics, 2004, 175, 829-834.	1.3	42
137	Pressure-induced instabilities in bulk TiO2rutile. Journal of Physics Condensed Matter, 2004, 16, 273-292.	0.7	42
138	Orthorhombic distortion on Li intercalation in anatase. Physical Review B, 2004, 69, .	1.1	71
139	Metal-insulator and magnetic transition of NiO at high pressures. Physical Review B, 2004, 69, .	1.1	60
140	Electronic and magnetic structure ofLaMnO3from hybrid periodic density-functional theory. Physical Review B, 2004, 69, .	1.1	116
141	A new phase of lithiated titania predicted from first principles. Chemical Physics Letters, 2003, 371, 150-156.	1.2	30
142	Surface to bulk charge transfer at an alkali metal/metal oxide interface. Surface Science, 2003, 547, L859-L864.	0.8	22
143	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
144	The structure of higher defective ZnO (101Ì„0). Surface Science, 2003, 529, L281-L284.	0.8	16

#	Article	IF	Citations
145	Diffusion of Li-ions in rutile. An ab initio study. Solid State Ionics, 2003, 157, 35-38.	1.3	113
146	Stability of rocksalt polar surfaces:â€‚â€‚Anab initiostudy of MgO(111) and NiO(111). Physical Review B, 2003, 68, .	1.1	116
147	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
148	Density-functional simulations of lithium intercalation in rutile. Physical Review B, 2002, 65, .	1.1	110
149	New ultrasoft pseudopotentials for the study of silicates. Molecular Simulation, 2002, 28, 213-237.	0.9	9
150	Phase Transformations of Anatase TiO2 on Cation Intercalation from First Principles Simulation.. Materials Research Society Symposia Proceedings, 2002, 731, 351.	0.1	3
151	First-principles calculations of the phase stability ofTiO2. Physical Review B, 2002, 65, .	1.1	464
152	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
153	Structural deformations in lithium doped titanium dioxide. Computational Materials Science, 2002, 24, 235-240.	1.4	22
154	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
155	Lattice dynamics of TiO2 rutile: influence of gradient corrections in density functional calculations. Chemical Physics Letters, 2002, 364, 528-534.	1.2	132
156	Effect of Diffusion on Lithium Intercalation in Titanium Dioxide. Physical Review Letters, 2001, 86, 1275-1278.	2.9	215
157	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
158	Stability of Polar Oxide Surfaces. Physical Review Letters, 2001, 86, 3811-3814.	2.9	400
159	The structure of the reduced rutile TiO2(100) 1Ã—3 reconstruction. Surface Science, 2001, 479, L375-L381.	0.8	24
160	An ab Initio Study of Hydrogen Adsorption on ZnO(101Ì„0). Journal of Physical Chemistry B, 2001, 105, 6191-6193.	1.2	43
161	Analytical Hartree-Fock gradients for periodic systems. International Journal of Quantum Chemistry, 2001, 82, 1-13.	1.0	280
162	First principles simulation of surfaces and interfaces. Computer Physics Communications, 2001, 137, 59-73.	3.0	9

#	Article	IF	Citations
163	The structural relaxation of the Î±-Al2O3(0001) â€“ an investigation of potential errors. Chemical Physics Letters, 2001, 341, 412-418.	1.2	54
164	On the prediction of band gaps from hybrid functional theory. Chemical Physics Letters, 2001, 342, 397-401.	1.2	837
165	The hardest known oxide. Nature, 2001, 410, 653-654.	13.7	316
166	Theoretical study of chlorine adsorption on the Ag(111) surface. Physical Review B, 2001, 63, .	1.1	57
167	Analytical Hartreeâ€“Fock gradients for periodic systems. , 2001, 82, 1.		7
168	Chlorine adsorption on the Cu(111) surface. Chemical Physics Letters, 2000, 317, 282-289.	1.2	120
169	An ab initio study of ZnO(101Ì„0). Surface Science, 2000, 457, L342-L346.	0.8	136
170	An ab initio study of Î±-Al2O3(0001): the effects of exchange and correlation functionals. Surface Science, 2000, 458, 25-33.	0.8	52
171	An ab-initio study of ZnO(112Ì„0). Surface Science, 2000, 468, L851-L855.	0.8	86
172	The physical and electronic structure of the rutile (001) surface. Surface Science, 2000, 446, 119-127.	0.8	41
173	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
174	First-principles study of potassium adsorption onTiO2surfaces. Physical Review B, 1999, 59, 15457-15463.	1.1	59
175	The influence of soft vibrational modes on our understanding of oxide surface structure. Faraday Discussions, 1999, 114, 305-312.	1.6	106
176	A density functional study of lithium bulk and surfaces. Journal of Physics Condensed Matter, 1999, 11, 5007-5019.	0.7	74
177	New Vistas for First-Principles Simulation. , 1999, , 137-146.		0
178	The electronic structure of Si(100) 2 Ã— 1î—¸Cl: reinterpreting ARP measurements. Surface Science, 1998, 398, 301-307.	0.8	8
179	Mixed Dissociative and Molecular Adsorption of Water on the Rutile (110) Surface. Physical Review Letters, 1998, 80, 762-765.	2.9	310
180	An experimental and theoretical investigation of the electronic structure of CdO. Journal of Physics Condensed Matter, 1998, 10, 8447-8458.	0.7	68

#	Article	IF	Citations
181	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
182	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
183	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
184	Anab initio Hartreeâ€“Fock study of Î±-MoO3. Journal of Materials Chemistry, 1997, 7, 959-967.	6.7	96
185	Ab initio simulation of molecular processes on oxide surfaces. Faraday Discussions, 1997, 106, 135-154.	1.6	69
186	Molecular dynamics study of the high temperature fusion of TiO2 nanoclusters. Journal of Materials Chemistry, 1997, 7, 2543-2546.	6.7	16
187	First-principles spin-polarized calculations on the reduced and reconstructedTiO2(110) surface. Physical Review B, 1997, 55, 15919-15927.	1.1	191
188	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
189	An ab initio study of the magnetic coupling in bi-metallic CrIII cyanides. Chemical Physics Letters, 1997, 266, 507-511.	1.2	17
190	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
191	The TiO2(100)(1 Ã— 3) reconstruction: insights from ab initio calculations. Surface Science, 1996, 364, 431-438.	0.8	52
192	Direct evidence of O(p) holes in Li-doped NiO from Hartree-Fock calculations. Chemical Physics Letters, 1996, 250, 66-70.	1.2	56
193	Structure of the Î±-Cr2O3(0001) surface: Anab initiototal-energy study. Physical Review B, 1996, 54, 14066-14070.	1.1	80
194	Molecular dynamics study of TiO2 microclusters. Journal of Materials Chemistry, 1996, 6, 1385.	6.7	38
195	An ab initio Hartree-Fock investigation of galena (PbS). Chemical Physics Letters, 1996, 257, 627-632.	1.2	38
196	First-principles molecular dynamics simulation of water dissociation on TiO2 (110). Chemical Physics Letters, 1996, 261, 246-252.	1.2	160
197	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
198	First principles simulation of oxide materials. Acta Crystallographica Section A: Foundations and Advances, 1996, 52, C92-C92.	0.3	0

#	Article	IF	Citations
199	Ab initiostudy of the surface and interfacial properties of a layered MgO/NiO film. Physical Review B, 1995, 52, 5375-5384.	1.1	35
200	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
201	A super-cell approach for the study of localized defects in solids: carbon substitution in bulk silicon. Journal of Physics Condensed Matter, 1994, 6, 8573-8583.	0.7	9
202	Ab initiodetermination of the bulk properties of MgO. Physical Review B, 1994, 49, 8574-8582.	1.1	96
203	Ab initio study of ZnO (101Â¯0) surface relaxation. Physical Review B, 1994, 49, 11153-11158.	1.1	92
204	Water chemistry on surface defect sites: Chemidissociation versus physisorption on MgO(001). Journal of Chemical Physics, 1994, 101, 1547-1554.	1.2	189
205	Ab initio study of high pressure phase transition in GaN. Journal of Physics and Chemistry of Solids, 1994, 55, 1357-1361.	1.9	99
206	Ab initiostudy of MnO and NiO. Physical Review B, 1994, 50, 5041-5054.	1.1	441
207	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
208	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
209	The Derivation of Shell Model Potentials for MgCl₂FromAb InitioTheory. Molecular Simulation, 1992, 9, 171-174.	0.9	18
210	Correlation functional estimates of the dispersion intraction in semi-ionic compounds. Journal of Physics Condensed Matter, 1992, 4, L261-L264.	0.7	12
211	The structural properties of beta -MgCl2; an ab initio study. Journal of Physics Condensed Matter, 1992, 4, 3873-3882.	0.7	34
212	Electrons in partially ordered alloys-Ag0.5Zn0.5. Journal of Physics Condensed Matter, 1989, 1, 3315-3324.	0.7	6
213	An XPS investigation of the electronic structure in AgZn. European Physical Journal B, 1989, 75, 291-295.	0.6	5
214	Structure and Interactions at the Mg(0001)/Water Interface: An ab initio Study. Journal of Chemical Physics, 0, , .	1.2	2