# Graeme W Watson

## List of Publications by Year in Descending Order



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|---|---|---|---|
| 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 | Defect chemistry of LaGaO3 doped with divalent cations. *Solid State Ionics*, **2022**, 374, 115828 | 3.3 | 0 |
| 217 | Modulating Structural and Electronic Properties of Rare Archimedean and Johnson-Type Mn Cages. *Inorganic Chemistry*, **2021**, 60, 8388-8393 | 5.1 | 0 |
| 216 | J2suscep: Calculation of magnetic exchange coupling and temperature dependence of magnetic susceptibility. *Journal of Open Source Software*, **2021**, 6, 2838 | 5.2 | 1 |
| 215 | A computational study of the electrochemical cyanide reduction for ambient ammonia production on a nickel cathode. *Catalysis Science and Technology*, **2021**, 11, 5633-5640 | 5.5 | |
| 214 | Altering the nature of coupling by changing the oxidation state in a {Mn} cage. *Dalton Transactions*, **2020**, 49, 8086-8095 | 4.3 | 2 |
| 213 | A cubane-type manganese complex with H2O oxidation capabilities. *Sustainable Energy and Fuels*, **2020**, 4, 4464-4468 | 5.8 | 5 |
| 212 | Aggregation induced emission (AIE) active 4-amino-1,8-naphthalimide-Tröger's base for the selective sensing of chemical explosives in competitive aqueous media. *Chemical Communications*, **2020**, 56, 2562-2565 | 5.8 | 32 |
| 211 | Computational modelling of solid oxide fuel cells. *Current Opinion in Electrochemistry*, **2020**, 21, 14-21 | 7.2 | 7 |
| 210 | Computationally Driven Discovery of Layered Quinary Oxychalcogenides: Potential -Type Transparent Conductors?. *Matter*, **2020**, 3, 759-781 | 12.7 | 5 |
| 209 | Hyper-crosslinked 4-amino-1,8-naphthalimide Tröger's base containing pyridinium covalent organic polymer (COP) for discriminative fluorescent sensing of chemical explosives. *Supramolecular Chemistry*, **2020**, 32, 508-517 | 1.8 | 2 |
| 208 | The structure and electronic structure of tin oxides **2020**, 11-39 | | 2 |
| 207 | "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 |
| 206 | Quasiparticle Calculations on Lead-Free Hybrid Germanium Iodide Perovskite CHNHGeI for Photovoltaic Applications. *ACS Omega*, **2019**, 4, 5661-5669 | 3.9 | 15 |
| 205 | Layered CeSO and LiCeSO Oxide Chalcogenides Obtained via Topotactic Oxidative and Reductive Transformations. *Inorganic Chemistry*, **2019**, 58, 3838-3850 | 5.1 | 3 |
| 204 | Flexible Metal-Organic Frameworks for Light-Switchable CO Sorption Using an Auxiliary Ligand Strategy. *Inorganic Chemistry*, **2019**, 58, 9766-9772 | 5.1 | 5 |
| 203 | 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 |
| 202 | Defects in orthorhombic LaMnO - ionic versus electronic compensation. *Physical Chemistry Chemical Physics*, **2018**, 20, 19257-19267 | 3.6 | 2 |

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|---|---|---|---|
| 201 | Photocatalysis: Evidence and Effect of Photogenerated Charge Transfer for Enhanced Photocatalysis in WO3/TiO2 Heterojunction Films: A Computational and Experimental Study (Adv. Funct. Mater. 18/2017). *Advanced Functional Materials*, **2017**, 27, | 15.6 | 1 |
| 200 | Modelling the electronic structure of orthorhombic LaMnO3. *Solid State Ionics*, **2017**, 299, 13-17 | 3.3 | 17 |
| 199 | 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 |
| 198 | Modelling oxygen defects in orthorhombic LaMnO and its low index surfaces. *Physical Chemistry Chemical Physics*, **2017**, 19, 24636-24646 | 3.6 | 16 |
| 197 | The importance of polarizability in the modeling of ionic diffusion in ceria. *IOP Conference Series: Materials Science and Engineering*, **2017**, 169, 012002 | 0.4 | 0 |
| 196 | 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 |
| 195 | Reversible adsorption and storage of secondary explosives from water using a Tr□ger's base-functionalised polymer. *Journal of Materials Chemistry A*, **2017**, 5, 25014-25024 | 13 | 22 |
| 194 | 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 |
| 193 | Modelling potential photovoltaic absorbers Cu3MCh4(M = V, Nb, Ta; Ch = S, Se, Te) using density functional theory. *Journal of Physics Condensed Matter*, **2016**, 28, 175801 | 1.8 | 10 |
| 192 | Assessing the potential of Mg-doped Cr□□ as a novel p-type transparent conducting oxide. *Journal of Physics Condensed Matter*, **2016**, 28, 125501 | 1.8 | 16 |
| 191 | Identification of metal s states in Sn-doped anatase by polarisation dependent hard X-ray photoelectron spectroscopy. *Chemical Physics Letters*, **2016**, 647, 59-63 | 2.5 | 4 |
| 190 | Correlating Lithium Hydroxyl Accumulation with Capacity Retention in V2O5 Aerogel Cathodes. *ACS Applied Materials & Interfaces*, **2016**, 8, 11532-8 | 9.5 | 19 |
| 189 | Structure and Reducibility of CeO2 Doped with Trivalent Cations. *Journal of Physical Chemistry C*, **2016**, 120, 23430-23440 | 3.8 | 49 |
| 188 | Electronic and surface properties of Ga-doped In2O3 ceramics. *Applied Surface Science*, **2015**, 349, 970-982 | 3.7 | 25 |
| 187 | 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 |
| 186 | Strain effects on the ionic conductivity of Y-doped ceria: A simulation study. *Journal of Electroceramics*, **2014**, 32, 28-36 | 1.5 | 28 |
| 185 | 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 |
| 184 | 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 |

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| 183 | 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 |
| 182 | Understanding doping anomalies in degenerate p-type semiconductor LaCuOSe. *Journal of Materials Chemistry C*, **2014**, 2, 3429-3438 | 7.1 | 45 |
| 181 | The electronic structure of silver orthophosphate: experiment and theory. *Journal of Materials Chemistry A*, **2014**, 2, 6092-6099 | 13 | 18 |
| 180 | The electronic structure of the antimony chalcogenide series: Prospects for optoelectronic applications. *Journal of Solid State Chemistry*, **2014**, 213, 116-125 | 3.3 | 68 |
| 179 | Occupation matrix control of d- and f-electron localisations using DFT + U. *Physical Chemistry Chemical Physics*, **2014**, 16, 21016-31 | 3.6 | 105 |
| 178 | Ceria co-doping: synergistic or average effect?. *Physical Chemistry Chemical Physics*, **2014**, 16, 8320-31 | 3.6 | 60 |
| 177 | The nature of oxygen states on the surfaces of CeO2 and La-doped CeO2. *Chemical Physics Letters*, **2014**, 608, 239-243 | 2.5 | 25 |
| 176 | Valence-band density of states and surface electron accumulation in epitaxial SnO2 films. *Physical Review B*, **2014**, 90, | 3.3 | 50 |
| 175 | Electronic Structures of Antimony Oxides. *Journal of Physical Chemistry C*, **2013**, 117, 14759-14769 | 3.8 | 62 |
| 174 | Band alignment of rutile and anatase TiO*Nature Materials*, **2013**, 12, 798-801 | 27 | 1656 |
| 173 | Computational testing of trivalent dopants in CeO2 for improved high-dielectric behaviour. *Journal of Materials Chemistry C*, **2013**, 1, 1093-1098 | 7.1 | 30 |
| 172 | Understanding the defect chemistry of tin monoxide. *Journal of Materials Chemistry C*, **2013**, 1, 8194 | 7.1 | 59 |
| 171 | Effects of Li-ion vacancies on the ionic conduction mechanism of LiMgSO4F. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 074003 | 2 | 2 |
| 170 | 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 |
| 169 | Chemical Expansion in SOFC Materials: Ramifications, Origins, and Mitigation. *ECS Transactions*, **2013**, 57, 643-648 | 1 | 2 |
| 168 | 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 |
| 167 | Convergence of density and hybrid functional defect calculations for compound semiconductors. *Physical Review B*, **2013**, 88, | 3.3 | 77 |
| 166 | Band gap engineering of In2O3 by alloying with Tl2O3. *Applied Physics Letters*, **2013**, 103, 262108 | 3.4 | 18 |

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| 165 | Reducing the chemical expansion coefficient in ceria by addition of zirconia. *Energy and Environmental Science*, **2013**, 6, 1142 | 35.4 | 40 |
| 164 | PbO2: from semi-metal to transparent conducting oxide by defect chemistry control. *Chemical Communications*, **2013**, 49, 448-50 | 5.8 | 23 |
| 163 | The band structure of WO3 and non-rigid-band behaviour in Na0.67WO3 derived from soft x-ray spectroscopy and density functional theory. *Journal of Physics Condensed Matter*, **2013**, 25, 165501 | 1.8 | 7 |
| 162 | Electronic Structure of Epitaxial Sn-Doped Anatase Grown on SrTiO3(001) by Dip Coating. *Journal of Physical Chemistry C*, **2013**, 117, 15221-15228 | 3.8 | 9 |
| 161 | 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 |
| 160 | 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 |
| 159 | Energy-band alignment of II-VI/Zn3P2 heterojunctions from x-ray photoemission spectroscopy. *Journal of Applied Physics*, **2013**, 113, 203705 | 2.5 | 23 |
| 158 | Cooperative Mechanism for the Diffusion of Li+ Ions in LiMgSO4F. *Journal of Physical Chemistry C*, **2012**, 116, 18618-18625 | 3.8 | 40 |
| 157 | The synthesis and characterisation of novel ferrocenyl polyphenylenes. *Dalton Transactions*, **2012**, 41, 8850-60 | 4.3 | 28 |
| 156 | Oxygen Vacancy Ordering and the Conductivity Maximum in Y2O3-Doped CeO2. *Chemistry of Materials*, **2012**, 24, 222-229 | 9.6 | 91 |
| 155 | Scanlon and Watson Reply:. *Physical Review Letters*, **2012**, 108, | 7.4 | 1 |
| 154 | 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 |
| 153 | On the possibility of p-type SnO2. *Journal of Materials Chemistry*, **2012**, 22, 25236 | | 134 |
| 152 | Computational study of the proton affinity and basicity of structurally diverse □-adrenoceptor ligands. *Journal of Physical Organic Chemistry*, **2012**, 25, 351-360 | 2.1 | 4 |
| 151 | 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 |
| 150 | Charge localization increases chemical expansion in cerium-based oxides. *Physical Chemistry Chemical Physics*, **2012**, 14, 12070-4 | 3.6 | 61 |
| 149 | Electronic structures of silver oxides. *Physical Review B*, **2011**, 84, | 3.3 | 51 |
| 148 | Understanding the p-type defect chemistry of CuCrO2. *Journal of Materials Chemistry*, **2011**, 21, 3655 | | 163 |

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| 147 | 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 |
| 146 | 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 |
| 145 | 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 |
| 144 | Uncovering the complex behavior of hydrogen in Cu2O. *Physical Review Letters*, **2011**, 106, 186403 | 7.4 | 46 |
| 143 | Stereochemistry of post-transition metal oxides: revision of the classical lone pair model. *Chemical Society Reviews*, **2011**, 40, 4455-63 | 58.5 | 456 |
| 142 | Role of Lithium Ordering in the LixTiO2 Anatase -> Titanate Phase Transition. *Journal of Physical Chemistry Letters*, **2011**, 2, 1657-1661 | 6.4 | 38 |
| 141 | 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 |
| 140 | Comparison of the defective pyrochlore and ilmenite polymorphs of AgSbO3 using GGA and hybrid DFT. *Physical Review B*, **2011**, 83, | 3.3 | 23 |
| 139 | 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 |
| 138 | Role of Lattice Distortions in the Oxygen Storage Capacity of Divalently Doped CeO2. *Chemistry of Materials*, **2011**, 23, 4464-4468 | 9.6 | 158 |
| 137 | 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 |
| 136 | Chemical bonding in copper-based transparent conducting oxides: CuMO2 (M = In, Ga, Sc). *Journal of Physics Condensed Matter*, **2011**, 23, 334201 | 1.8 | 22 |
| 135 | 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 |
| 134 | Comment on Generalized Gradient Approximation +UStudy for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxide *Japanese Journal of Applied Physics*, **2011**, 50, 069101 | 1.4 | 1 |
| 133 | Nature of the band gap of Tl2O3. *Physical Review B*, **2011**, 83, | 3.3 | 37 |
| 132 | Comment on Generalized Gradient Approximation +UStudy for Metallization Mechanism of Niobium-Doped Anatase Titanium Dioxide *Japanese Journal of Applied Physics*, **2011**, 50, 069101 | 1.4 | |
| 131 | Understanding conductivity anomalies in Cu(I)-based delafossite transparent conducting oxides: Theoretical insights. *Journal of Chemical Physics*, **2010**, 132, 024707 | 3.9 | 93 |
| 130 | Conductivity Limits in CuAlO2 from Screened-Hybrid Density Functional Theory. *Journal of Physical Chemistry Letters*, **2010**, 1, 3195-3199 | 6.4 | 102 |

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| 129 | 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 |
| 128 | Undoped n-Type Cu2O: Fact or Fiction?. *Journal of Physical Chemistry Letters*, **2010**, 1, 2582-2585 | 6.4 | 111 |
| 127 | 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 |
| 126 | GGA+U description of lithium intercalation into anatase TiO2. *Physical Review B*, **2010**, 82, | 3.3 | 93 |
| 125 | Electronic structure of mixed-valence silver oxide AgO from hybrid density-functional theory. *Physical Review B*, **2010**, 81, | 3.3 | 64 |
| 124 | Theoretical and Experimental Study of the Electronic Structures of MoO3 and MoO2. *Journal of Physical Chemistry C*, **2010**, 114, 4636-4645 | 3.8 | 435 |
| 123 | Understanding conductivity in SrCu2O2: stability, geometry and electronic structure of intrinsic defects from first principles. *Journal of Materials Chemistry*, **2010**, 20, 1086-1096 | | 39 |
| 122 | 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 |
| 121 | Testing Interatomic Potentials for QM/MM Embedded-Cluster Calculations on Ceria Surfaces. *E-Journal of Surface Science and Nanotechnology*, **2009**, 7, 413-420 | 0.7 | 8 |
| 120 | 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 |
| 119 | Polaronic trapping of electrons and holes by native defects in anatase TiO2. *Physical Review B*, **2009** , 80, | 3.3 | 222 |
| 118 | Comparative study of bandwidths in copper delafossites from x-ray emission spectroscopy. *Physical Review B*, **2009**, 80, | 3.3 | 33 |
| 117 | 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 |
| 116 | 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 |
| 115 | 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 |
| 114 | (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 |
| 113 | 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 |
| 112 | Energetic and Electronic Structure Analysis of Intrinsic Defects in SnO2. *Journal of Physical Chemistry C*, **2009**, 113, 439-448 | 3.8 | 236 |

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|---|---|---|---|
| 111 | Acceptor levels in p-type Cu(2)O: rationalizing theory and experiment. *Physical Review Letters*, **2009**, 103, 096405 | 7.4 | 237 |
| 110 | Small polarons in Nb- and Ta-doped rutile and anatase TiO2. *Journal of Materials Chemistry*, **2009**, 19, 5175 | | 143 |
| 109 | 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 |
| 108 | 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 |
| 107 | X-ray spectroscopic study of the electronic structure of CuCrO2. *Physical Review B*, **2009**, 79, | 3.3 | 82 |
| 106 | Effect of Cr substitution on the electronic structure of CuAl1□CrxO2. *Physical Review B*, **2009**, 79, | 3.3 | 102 |
| 105 | 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 |
| 104 | Competing Defect Mechanisms and Hydrogen Adsorption on Li-Doped MgO Low Index Surfaces: A DFT+U Study. *E-Journal of Surface Science and Nanotechnology*, **2009**, 7, 395-404 | 0.7 | 9 |
| 103 | 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 |
| 102 | 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 |
| 101 | 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 |
| 100 | Selective formation of the rctt chair stereoisomers of octa-O-alkyl resorcin[4]arenes using Br□sted acid catalysis. *New Journal of Chemistry*, **2008**, 32, 994 | 3.6 | 12 |
| 99 | Ultrafast IR spectroscopy of the short-lived transients formed by UV excitation of cytosine derivatives. *Chemical Communications*, **2007**, 2130-2 | 5.8 | 38 |
| 98 | Atomistic modeling of multilayered ceria nanotubes. *Nano Letters*, **2007**, 7, 543-6 | 11.5 | 32 |
| 97 | Polymorphism in Bismuth Stannate: A First-Principles Study. *Chemistry of Materials*, **2007**, 19, 5158-5164 | 9.6 | 40 |
| 96 | Experimental and theoretical study of the electronic structures of □PbO and □PbO2. *Journal of Materials Chemistry*, **2007**, 17, 267-277 | | 92 |
| 95 | 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 |
| 94 | A DFT+U description of oxygen vacancies at the TiO2 rutile (110) surface. *Surface Science*, **2007**, 601, 5034-5041 | 1.8 | 410 |

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|---|---|---|---|
| 93 | 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 |
| 92 | Nature of electronic states at the Fermi level of metallic PbO2 revealed by hard x-ray photoemission spectroscopy. *Physical Review B*, **2007**, 75, | 3.3 | 36 |
| 91 | Vibrational properties of CO on ceria surfaces. *Surface Science*, **2006**, 600, 175-178 | 1.8 | 42 |
| 90 | The surface dependence of CO adsorption on Ceria. *Journal of Physical Chemistry B*, **2006**, 110, 16600-6 | 3.4 | 157 |
| 89 | Reduction of NO2 on ceria surfaces. *Journal of Physical Chemistry B*, **2006**, 110, 2256-62 | 3.4 | 115 |
| 88 | Application of molecular dynamics DL_POLY codes to interfaces of inorganic materials. *Molecular Simulation*, **2006**, 32, 1079-1093 | 2 | 16 |
| 87 | Simulation of the structure of organosilane film coatings. *Molecular Simulation*, **2006**, 32, 1095-1101 | 2 | 2 |
| 86 | CeO2 catalysed conversion of CO, NO2 and NO from first principles energetics. *Physical Chemistry Chemical Physics*, **2006**, 8, 216-8 | 3.6 | 98 |
| 85 | 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 |
| 84 | 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 |
| 83 | 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 |
| 82 | A theoretical and experimental study of the distorted pyrochlore Bi2Sn2O7. *Journal of Materials Chemistry*, **2006**, 16, 3452 | | 27 |
| 81 | Hydrogen adsorption and diffusion on Pt {111} and PtSn {111}. *Journal of Materials Chemistry*, **2006**, 16, 1989 | | 36 |
| 80 | Hole localization in Al doped silica: A DFT + U description. *Journal of Chemical Physics*, **2006**, 125, 144701 | 3.9 | 101 |
| 79 | Theoretical proton affinities of alpha1 adrenoceptor ligands. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 1580-7 | 3.4 | 11 |
| 78 | Oxygen vacancy formation and migration in ceria. *Solid State Ionics*, **2006**, 177, 3069-3074 | 3.3 | 256 |
| 77 | Asymmetric acyl-transfer promoted by readily assembled chiral 4-N,N-dialkylaminopyridine derivatives. *Organic and Biomolecular Chemistry*, **2006**, 4, 2785-93 | 3.9 | 50 |
| 76 | 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 |

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|---|---|---|---|
| 75 | 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 |
| 74 | Experimental and theoretical study of the electronic structure of HgO and Tl2O3. *Physical Review B*, **2005**, 71, | 3.3 | 48 |
| 73 | Computer aided design of nano-structured materials with tailored ionic conductivities. *Physical Chemistry Chemical Physics*, **2005**, 7, 16-8 | 3.6 | 22 |
| 72 | Comparative molecular dynamics simulations of uncomplexed, 'agonist-bound' and 'antagonist-bound' alpha1A adrenoceptor models. *Biochemical and Biophysical Research Communications*, **2005**, 333, 737-41 | 3.4 | 4 |
| 71 | 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 |
| 70 | The electronic structure of oxygen vacancy defects at the low index surfaces of ceria. *Surface Science*, **2005**, 595, 223-232 | 1.8 | 585 |
| 69 | Why is lead dioxide metallic?. *Chemical Physics Letters*, **2005**, 411, 181-185 | 2.5 | 59 |
| 68 | 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 |
| 67 | Modelling the interaction of catecholamines with the alpha 1A adrenoceptor towards a ligand-induced receptor structure. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 357-67 | 4.2 | 2 |
| 66 | Electronic structures of rocksalt, litharge, and herzenbergite SnO by density functional theory. *Physical Review B*, **2004**, 70, | 3.3 | 105 |
| 65 | Modelling Inorganic Solids and Their Interfaces: A Combined Approach of Atomistic and Electronic Structure Simulation Techniques. *ChemInform*, **2004**, 35, no | | 1 |
| 64 | On the involvement of the shallow core 5d level in the bonding in HgO. *Chemical Physics Letters*, **2004**, 399, 98-101 | 2.5 | 25 |
| 63 | Microwave induced preparation of a-axis oriented double-ended needle-shaped ZnO microparticles. *Chemical Communications*, **2004**, 2294-5 | 5.8 | 50 |
| 62 | Computational development of an alpha1A-adrenoceptor model in a membrane mimic. *Biochemical and Biophysical Research Communications*, **2004**, 324, 916-21 | 3.4 | 12 |
| 61 | Re-evaluation of the adsorption mode of ethene on the {111} surface of palladium using density functional theory. *Surface Science*, **2003**, 547, L853-L858 | 1.8 | 6 |
| 60 | 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 |
| 59 | Synthesis, structure and ionic conductivity in nanopolycrystalline BaF2/CaF2 heterolayers. *Chemical Communications*, **2003**, 1804-6 | 5.8 | 15 |
| 58 | Metal oxide encapsulated nanoparticles. *Journal of Materials Chemistry*, **2003**, 13, 2078 | | 4 |

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| 57 | Sulfonylation of substituted benzenes using Zn-exchanged zeolites. *Journal of Molecular Catalysis A* , **2002**, 178, 205-209 | | 14 |
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| 55 | Atomistic Structures of 25 000-Atom Oxide Nanoparticles Supported on an Oxide Substrate. *Journal of Physical Chemistry B*, **2002**, 106, 10793-10807 | 3.4 | 11 |
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