

516 Pre-2015 Publications that utilised HEC resources

46 papers acknowledge [\[EP/D504872\]](#), [339 \[EP/F067496\]](#), and [060 \[EP/L000202\]](#)

Typically work performed on [HPCx](#) (IBM), [HECToR](#) (CRAY) and [ARCHER](#) (CRAY) HEC platforms; the DOI references are active links to publications via <http://dx.doi.org> and [#] direct links to pdf documents for members.

From Jochen Blumberger's Group

[\[1\] Free energies for biological electron transfer from QM/MM calculations: method, application and critical assessment,](#)

J. Blumberger,

Phys. Chem. Chem. Phys. (2008) 10, 5651-5667; DOI: 10.1039/b807444e

[\[2\] \$\text{Cu}^+_{\text{aq}}/\text{Cu}^{2+}_{\text{aq}}\$ redox reaction exhibits non-linear solvent response due to change in coordination number,](#)

J. Blumberger,

J. Am. Chem. Soc. (2008) 130, 16065-16068; DOI: 10.1021/ja805471a

[\[3\] Charge constrained density functional molecular dynamics for simulation of condensed phase electron transfer reactions,](#)

H. Oberhofer and J. Blumberger,

J. Chem. Phys. (2009) 131, 064101-064111; DOI: 10.1063/1.3190169

[\[4\] Single-ion reorganization free energy of aqueous \$\text{Ru}\(\text{bpy}\)_3^{2+/3+}\$ and \$\text{Ru}\(\text{H}_2\text{O}\)_6^{2+/3+}\$ from photoemission spectroscopy and density functional based molecular dynamics simulation,](#)

R. Seidel, M. Faubel, B. Winter and J. Blumberger,

J. Am. Chem. Soc. (2009) 131, 16127-16137; DOI: 10.1021/ja9047834

[\[5\] Insight into the mechanism of the \$\text{Ru}^{2+}\$ - \$\text{Ru}^{3+}\$ electron self-exchange reaction from quantitative rate calculations,](#)

H. Oberhofer and J. Blumberger,

Angew. Chem. Int. Ed. (2010) 49, 3631-3634; DOI: 10.1002/anie.200906455

[\[6\] Energy levels and redox properties of aqueous \$\text{Mn}^{2+/3+}\$ from photoemission spectroscopy and density functional based molecular dynamics,](#)

J. Moens, R. Seidel, P. Geerlings, M. Faubel, B. Winter and J. Blumberger,

J. Phys. Chem. B (2010) 114, 9173-9182; DOI: 10.1021/jp101527v

[\[7\] Prediction of reorganization free energies for biological electron transfer: A comparative study of Ru-modified proteins and a 4-helix bundle protein,](#)

V. Tipmanee, H. Oberhofer, M. Park, K. S. Kim and J. Blumberger,

J. Am. Chem. Soc. (2010) 132, 17032-17040; DOI: 10.1021/ja107876p

[\[8\] Electronic coupling matrix elements from charge constrained density functional theory calculations using a plane wave basis set,](#)

H. Oberhofer and J. Blumberger,

J. Chem. Phys. (2010) 133, 244105-244114; DOI: 10.1063/1.3507878

[\[9\] Absolute pKa values and solvation structure of amino acids from density functional based molecular dynamics simulation,](#)

M. Mangold, L. Rolland, F. Constanzo, M. Sprik, M. Sulpizi and J. Blumberger,

J. Chem. Theor. Comput. (2011) 7, 1951-1961; DOI: 10.1021/ct100715x

[\[10\] Proton transfer drives protein radical formation in HP catalase but not in PV catalase,](#)

M. Alfonso-Prieto, H. Oberhofer, M. L. Klein, C. Rovira and J. Blumberger,

J. Am. Chem. Soc. (2011) 133, 4285-4298; DOI: 10.1021/ja1110706

[\[11\] Mechanistic insight into the blocking of CO diffusion in \[NiFe\]-hydrogenase mutants through multiscale simulation,](#)

P. Wang and J. Blumberger,

Proc. Natl. Acad. Sci. USA (2012) 109, 6399-6404; DOI: 10.1073/pnas.1121176109

[\[12\] Thermodynamics of electron flow in the bacterial deca-heme cytochrome MtrF,](#)

M. Breuer, P. Zarzycki, J. Blumberger and K.M. Rosso

J. Am. Chem. Soc. (2012) 134, 9868-9871; DOI: 10.1021/ja3027696

[\[13\] Revisiting electronic couplings and incoherent hopping models for electron transport in crystalline \$\text{C}_{60}\$ at ambient temperature,](#)

H. Oberhofer and J. Blumberger,

Phys. Chem. Chem. Phys. (2012) 14, 13846; DOI: 10.1039/c2cp41348e

[\[14\] Molecular structure and free energy landscape for electron transport in the decaheme cytochrome MtrF,](#)

M. Breuer, P. Zarzycki, L. Shi, T.A. Clarke, M. Edwards, J. Butt, D.J. Richardson, J.K. Fredrickson, J.M. Zachara, J. Blumberger and K.M. Rosso,
Biochem. Soc. Trans. (2012) 40, 6; DOI: 10.1042/BST20120139

[15] On the inapplicability of electron hopping models for the organic semiconductor phenyl-C61-butyrac acid methyl ester,

F. Gajdos, H. Oberhofer, M. Dupuis and J. Blumberger,
J. Phys. Chem. Lett. (2013) 4, 1012; DOI: 10.1021/jz400227c

[16] Uncovering a dynamically formed substrate access tunnel in carbon monoxide dehydrogenase/acetyl-CoA synthase,

P. Wang, M. Bruschi, L. de Gioia and J. Blumberger,
J. Am. Chem. Soc. (2013) 135, 9493; DOI: 10.1021/ja403110s

[17] Micro-focused X-ray diffraction characterisation of high-quality [6,6]-phenyl C61 butyric acid methyl ester single crystals without solvent impurities,

G. Paterno, A. Warren, J. Spencer, G. Evans, V. Garcia Sakai, J. Blumberger and F. Cacialli,
J. Mater. Chem. C (2013) 1, 5619; DOI: 10.1039/c3tc31075b

[18] Electron flow in multi-heme bacterial cytochromes is a balancing act between heme electronic interaction and redox potentials,

M. Breuer, K.M. Rosso, J. Blumberger,
Proc. Natl. Acad. Sci. (2014) 111, 611; DOI 10.1073/pnas.1316156111

[19] The oxidative inactivation of FeFe hydrogenase reveals the flexibility of the H-cluster,
V. Fourmond, C. Greco, K. Sybirna, C. Baffert, P.-H. Wang, P. Ezanno, M. Montefiori, M. Bruschi, I. Meynial-Salles, P. Soucaille, J. Blumberger, H. Bottin, L. De Gioia and C. Léger,
Nature Chem. (2014) 6, 336-342; DOI 10.1038/NCHEM.1892

[20] Electronic couplings for molecular charge transfer: benchmarking CDFT, FODFT, and FODFTB against high-level *ab initio* calculations,

A. Kubas, F. Hoffmann, A. Heck, H. Oberhofer, M. Elstner and J. Blumberger,
J. Chem. Phys. (2014) 140, 104105, 1-21; DOI 10.1063/1.4867077

[21] Aerobic damage to [FeFe]-hydrogenases: activation barriers for the chemical attachment of O₂,

A. Kubas, D. De Sancho, R.B. Best and J. Blumberger,
Angew. Chem. Int. Ed. (2014) 53, 4081-4084; DOI 10.1002/anie.201400534

From Richard Catlow's Group

[1] Structure and stability of the (001) α -quartz surface,

T.P.M. Goumans, A. Wander, W.A. Brown and C.R.A. Catlow,
Phys. Chem. Chem. Phys. (2007) 9, 2146–2152; DOI: 10.1039/b701176h

[2] The H₂-hydrogenation of ketones catalysed by ruthenium(II) complexes: A density functional theory study,

D. Di Tommaso, S.A. French and C.R.A. Catlow,
J. Molecular Struct.: THEOCHEM (2007) 812, 39–49; DOI: 10.1016/j.theochem.2007.02.029

[3] Silica grain catalysis of methanol formation,

T.P.M. Goumans, A. Wander, C.R.A. Catlow and W.A. Brown,
Mon. Not. R. Astron. Soc. (2007) 382, 1829–1832; DOI: 10.1111/j.1365-2966.2007.12491.x

[4] Formation of CO₂ on a carbonaceous surface: a quantum chemical study,

T.P.M. Goumans, M.A. Uppal and W.A. Brown,
Mon. Not. R. Astron. Soc. (2008) 384, 1158–1164; DOI: 10.1111/j.1365-2966.2007.12788.x

[5] Hydrogenation of CO on a silica surface: An embedded cluster approach,

T.P.M. Goumans, C.R.A. Catlow and W.A. Brown,
J. Chem. Phys. (2008) 128, 134709; DOI: 10.1063/1.2888933

[6] Computational study of the factors controlling enantioselectivity in ruthenium(II) hydrogenation catalysts,

D. Di Tommaso, S.A. French, A. Zanotti-Gerosa, F. Hancock, E.J. Palin, and C.R.A. Catlow,
Inorg. Chem. (2008) 47, 7, 2674-2687; DOI: 10.1021/ic701981v

[7] Structure, stability and work functions of the low index surfaces of pure indium oxide and Sn-doped indium oxide (ITO) from density functional theory,

A. Walsh and C.R.A. Catlow,
J. Mater. Chem. (2010) 20, 10438–10444; DOI: 10.1039/c0jm01816c

[8] Oxygen interstitial structures in close-packed metal oxides,

A.A. Sokol, A. Walsh and C.R.A. Catlow,
Chem. Phys. Lett. (2010) 492, 44–48; DOI: 10.1016/j.cplett.2010.04.029

[9] Photostimulated reduction processes in a titania hybrid metal-organic framework,

- A. Walsh,
Chem. Phys. Chem. (2010) 11, 2341–2344; DOI: 10.1002/cphc.201000306
- [10] Surface energies control the self-organization of oriented In_2O_3 nanostructures on cubic zirconia, K.H.L. Zhang, A. Walsh, C.R.A. Catlow, V.K. Lazarov and R.G. Egdell, *Nano Lett.* (2010) 10, 3740–3746; DOI: 10.1021/nl102403t
- [11] Control of the band-gap states of metal oxides by the application of epitaxial strain: The case of indium oxide,
A. Walsh, C.R.A. Catlow, K.H.L. Zhang and R.G. Egdell,
Phys. Rev. B (2011) 83, 161202; DOI: 10.1103/PhysRevB.83.161202
- [12] Strontium migration assisted by oxygen vacancies in SrTiO_3 from classical and quantum mechanical simulations,
A. Walsh, C.R.A. Catlow, A.G.H. Smith, A.A. Sokol and S. M. Woodley,
Phys. Rev. B (2011) 83, 220301; DOI: 10.1103/PhysRevB.83.220301
- [13] Free energy of defect formation: Thermodynamics of anion Frenkel pairs in indium oxide,
A. Walsh, C.R.A. Catlow, K.H.L. Zhang and R.G. Egdell,
Phys. Rev. B (2011) 83, 224105; DOI: 10.1103/PhysRevB.83.224105
- [14] Electron and hole stability in GaN and ZnO,
A. Walsh, C.R.A. Catlow, M. Miskufova and A.A. Sokol,
J. Phys.-Condensed Matt. (2011) 23, 334217; DOI: 10.1088/0953-8984/23/33/334217
- [15] Correlating enantioselectivity with activation energies in the asymmetric hydrogenation of acetophenone catalysed by noyori-type complexes,
H.-Y.T. Chen, D. Di Tommaso, G. Hogarth and C.R.A. Catlow,
Catal. Lett. (2011) 141, 1761–1766; DOI: 10.1007/s10562-011-0704-1
- [16] Oxygen adsorption and dissociation on yttria stabilized zirconia surfaces,
X. Xia, R.J. Oldman and C.R.A. Catlow,
J. Mat. Chem. (2012) 22, 8594-8612; DOI: 10.1039/c2jm16604f
- [17] Controlling bulk conductivity in topological insulators: Key role of anti-site defects,
D.O. Scanlon, P.D.C. King, R.P. Singh, A. de la Torre, S.M. Walker, G. Balakrishnan, F. Baumberger and C.R.A. Catlow,
Adv. Mat. (2012) 24, 2154-2158; DOI: 10.1002/adma.201200187
- [18] One-dimensional embedded cluster approach to modeling CdS nanowires,
J. Buckeridge, S.T. Bromley, A. Walsh, S.M. Woodley, C.R.A. Catlow and A.A. Sokol,
J. Chem. Phys. (2013) 139, 124101, 1-11; DOI: 10.1063/1.4820415
- [19] Band alignment of rutile and anatase TiO_2 ,
D.O. Scanlon, C.W. Dunnill, J. Buckeridge, S.A. Shevlin, A.J. Logsdail, S.M. Woodley, C.R.A. Catlow, M.J. Powell, R.G. Palgrave, I.P. Parkin, G.W. Watson, T.W. Keal, P. Sherwood, A. Walsh and A.A. Sokol,
Nature Materials (2013) 12, 798-801; DOI: 10.1038/nmat3697
- [20] Dynamical response and instability in ceria under lattice expansion,
J. Buckeridge, D.O. Scanlon, A. Walsh, C.R.A. Catlow and A.A. Sokol,
Phys. Rev. B (2013) 87, 214304, 1-10; DOI: 10.1103/PhysRevB.87.214304
- [21] Defect engineering of BaSnO_3 for high-performance transparent conducting oxide applications,
D.O. Scanlon,
Phys. Rev. B (2013) 87, 161201, 1-5; DOI: 10.1103/PhysRevB.87.161201
- [22] The band structure of WO_3 and non-rigid band behaviour in $\text{Na}_{0.67}\text{WO}_3$ derived from soft X-ray spectroscopy and density functional theory,
B. Chen, J. Laverock, L.F.J. Piper, A.R.H. Preston, S.W. Cho, A. DeMasi, K.E. Smith, D.O. Scanlon, G.W. Watson, R.G. Egdell, P.-A. Glans and J.-H. Guo,
J. Phys: Condens. Matt. (2013) 25, 165501, 1-10; DOI: 10.1088/0953-8984/25/16/165501
- [23] Elucidating the nature of pseudo Jahn-Teller distortions in Li_xMnPO_4 : combining density functional theory with soft and hard X-ray spectroscopy,
L.F.J. Piper, N.F. Quackenbush, S. Sallis, D.O. Scanlon, G.W. Watson, K.-W. Nam, X.-Q. Yang, K.E. Smith, F. Omenya, N.A. Chernova and M.S. Whittingham,
J. Phys. Chem. C (2013) 117, 10383-10396; DOI: 10.1021/jp3122374
- [24] Energy-band alignment of II-VI/ Zn_3P_2 heterojunctions from X-ray photoemission spectroscopy,
J.P. Bosco, D.O. Scanlon, G.W. Watson, N.S. Lewis and H.A. Atwater,
J. Appl. Phys. (2013) 113, 203705; DOI: 10.1063/1.4807646
- [25] La-doped BaSnO_3 – degenerate perovskite transparent conducting oxide: evidence from synchrotron X-ray spectroscopy,

S. Sallis, D.O. Scanlon, S.C. Chae, N.F. Quackenbush, D.A. Fischer, J.C. Woicik, J.-H. Guo, S.W. Cheong and L.F.J. Piper,
Appl. Phys. Lett. (2013) 103, 042105; DOI: 10.1063/1.4816511

[26] Growth, disorder, and physical properties of ZnSnN₂,
N. Feldberg, J.D. Aldous, W.M. Linhart, L.J. Phillips, K. Durose, P.A. Stampe, R.J. Kennedy, D.O. Scanlon, G. Vardar, R.L. Field III, T.Y. Jen, R.S. Goldman, T.D. Veal and S.M. Durbin,
Appl. Phys. Lett. (2013) 103, 042109; DOI: 10.1063/1.4816438

[27] The interaction of hydrogen with the (010) surfaces of Mg and Fe olivine as models for interstellar dust grains: a density functional theory study,
C.A. Downing, B. Ahmady and C.R.A. Catlow,
Phil. Trans. R. Soc. A (2013) 371, 20110592; DOI: 10.1098/rsta.2011.0592

[28] Convergence of density and hybrid functional defect calculations for compound semiconductors,
H. Peng, D.O. Scanlon, V. Stevanovic, J. Vidal, G.W. Watson and S. Lany,
Phys. Rev. B (2013) 88, 115201; DOI: 10.1103/PhysRevB.88.115201

[29] Growth and properties of GaSbBi alloys,
M.K. Rajpalke, W.M. Linhart, M. Birkett, K.M. Yu, D.O. Scanlon, J. Buckeridge, T.S. Jones, M.J. Ashwin and T.D. Veal,
Appl. Phys. Lett. (2013) 103, 142106; DOI: 10.1063/1.4824077

[30] Band gap engineering of In₂O₃ by alloying with Ti₂O₃,
D.O. Scanlon, A. Regoutz, R.G. Egdell, D.J. Morgan and G.W. Watson,
Appl. Phys. Lett. (2013) 103, 262108; DOI: 10.1063/1.4860986

[31] Automated procedure to determine the thermodynamic stability of a material and the range of chemical potentials necessary for its formation relative to competing phases and compounds,
J. Buckeridge, D.O. Scanlon, A. Walsh and C.R.A. Catlow,
Comp. Phys. Commun. (2014) 185, 330; DOI: 10.1016/j.cpc.2013.08.026

[32] N incorporation and associated localized vibrational modes in GaSb,
J. Buckeridge, D.O. Scanlon, T.D. Veal, M.J. Ashwin, A. Walsh and C.R.A. Catlow,
Phys. Rev. B (2014) 89, 014107; DOI: 10.1103/PhysRevB.89.014107

[33] Understanding doping anomalies in degenerate p-type semiconductor LaCuOSe,
D.O. Scanlon, J. Buckeridge, C.R.A. Catlow and G.W. Watson,
J. Mater. Chem. C (2014) 2, 3429; DOI: 10.1039/c4tc00096j

[34] Strain and orientation modulated bandgaps and effective masses of phosphorene nanoribbons,
X. Han, H. Morgan Stewart, S.A. Shevlin, C.R.A. Catlow and Z.X. Guo,
Nano Lett. (2014) 14, 4607-4614; DOI: 10.1021/nl501658d

[35] Combinatorial atmospheric pressure chemical vapor deposition of F:TiO₂; the relationship between photocatalysis and transparent conducting oxide properties,
A. Kafizas, N. Noor, P. Carmichael, D.O. Scanlon, C.J. Carmalt and I.P. Parkin,
Adv. Funct. Mater. (2014) 24, 1758; DOI: 10.1002/adfm.201301333

[36] Electronic structure and band alignment of zinc nitride, Zn₃N₂,
S.-H. Yu, A. Walsh, D.O. Scanlon and A. Soon,
RSC Adv. (2014) 4, 3306; DOI: 10.1039/c3ra46558f

[37] Understanding the electronic structure of IrO₂ using hard X-ray photoelectron spectroscopy and density-functional theory,
M. Kahk, C.G. Poll, F.E. Oropeza, J.M. Ablett, D. Céolin, J-P. Rueff, S. Agrestini, Y. Utsumi, K.D. Tsuei, Y.F. Liao, F. Borgatti, G. Panaccione, A. Regoutz, R.G. Egdell, B.J. Morgan, D.O. Scanlon and D.J. Payne,
Phys. Rev. Lett. (2014) 112, 117601; DOI: 10.1103/PhysRevLett.112.117601

[38] Designer titania-supported Au-Pd nanoparticles for efficient photocatalytic hydrogen production,
R. Su, R. Tiruvalam, A.J. Logsdail, Q. He, C.A. Downing, M.T. Jensen, N. Dimitratos, L. Kesavan, P.P. Wells, R. Bechstein, H.H. Jensen, S. Wendt, C.R.A. Catlow, C.J. Kiely, G.J. Hutchings and F. Besenbacher,
ACS Nano (2014) 8, 3490-3497; DOI: 10.1021/nn500963m

[39] The reactivity of CO₂ on the MgO(100) surface,
C.A. Downing, A.A. Sokol and C.R.A. Catlow,
Phys. Chem. Chem. Phys. (2014) 16, 184-195; DOI: 10.1039/c3cp53458h

*[40] The nature of the molybdenum surface in iron molybdate; the active phase in selective methanol oxidation,
C. Brookes, P.P. Wells, N. Dimitratos, W. Jones, E.K. Gibson, D.J. Morgan, G. Cibir, C. Nicklin, D. Mora-Fonz, D.O. Scanlon, C.R.A. Catlow, and M. Bowker,
J. Phys. Chem. C (2014) 118, 26155-26161; DOI:10.1021/jp5081753

From Jamieson Christie's Group

[1] [Ab initio molecular dynamics simulations of structural changes associated with the incorporation of fluorine in bioactive phosphate glasses](#),

J.K. Christie, R.I. Ainsworth and N.H. de Leeuw,
Biomaterials (2014) 35, 6164-6171, DOI: 10.1016/j.biomaterials.2014.04.032r

*[2] [On the structure of biomedical silver-doped phosphate-based glasses from molecular dynamics simulations](#),

R.I. Ainsworth, J.K. Christie and N.H. de Leeuw,
Phys. Chem. Chem. Phys. (2014) 16, 21135-21143; DOI: 10.1039/C4CP00574K

From George Darling's Group

[1] [Stabilization of a complex perovskite superstructure under ambient conditions: Influence of cation composition and ordering, and evaluation as an SOFC cathode](#),

A. Demont, M.S. Dyer, R. Sayers, M.F. Thomas, M. Tsiamsouri, H.N. Nui, G.R. Darling, A. Daoud-Aladine, J.B. Claridge and M.J. Rosseinsky,
Chem. Mater. (2010) 22, 6598-6615; DOI: 10.1021/cm102475n

[2] [Chemical bonding and atomic structure in \$Y_2O_3:ZrO_2-SrTiO_3\$ layered heterostructures](#),

M.S. Dyer, G.R. Darling, J.B. Claridge and M.J. Rosseinsky,
Angew. Chem. Int. Ed. (2012) 51, 3418-3422; DOI: 10.1002/anie.201108068

[3] [Computationally assisted identification of functional inorganic materials](#),

M.S. Dyer, C. Collins, D. Hodgeman, P.A. Chater, A. Demont, S. Romani, R. Sayers, M.F. Thomas, J.B. Claridge, G.R. Darling and M.J. Rosseinsky,
Science (2013) 340, 847-852; DOI: 10.1126/science.1226558

*[4] [Reported and predicted structures of \$Ba\(Co,Nb\)_{1-\delta}O_3\$ hexagonal perovskite phases](#),

K.A. Bradley, C. Collins, M. S. Dyer, J. B. Claridge, G. R. Darling and M.J. Rosseinsky,
Phys. Chem. Chem. Phys. (2014) 16, 21073; DOI: 10.1039/c4cp01542h

From Graeme Day's Group

[1] [Modular and predictable assembly of porous organic molecular crystals](#),

J.T.A. Jones, T. Hasell, X. Wu, J. Bacsá, K.E. Jelfs, M. Schmidtman, S.Y. Chong, D.J. Adams, A. Trewin, F. Schiffman, F. Cora, B. Slater, A. Steiner, G.M. Day and A.I. Cooper,
Nature (2011) 474, 367-371; DOI: 10.1038/nature10125

[2] [Large self-assembled chiral organic cages: Synthesis, structure, and shape persistence](#),

K.E. Jelfs, X. Wu, M. Schmidtman, J.T.A. Jones, J.E. Warren, D.J. Adams and A.I. Cooper,
Angew. Chem. Int. Ed. (2011) 50 (45), 10653-10656; DOI: 10.1002/anie.201105104

[3] [In silico design of supramolecules from their precursors: odd-even effects in cage-forming reactions](#),

K.E. Jelfs, E.G.B. Eden, J.L. Culshaw, S. Shakespeare, E.O. Pyzer-Knapp, H.P.G. Thompson, J. Bacsá, G.M. Day, D.J. Adams and A.I. Cooper,
J. Am. Chem. Soc. (2013) 135, 9307; DOI: 10.1021/ja404253j

[4] [Shape prediction for supramolecular organic nanostructures: \[4+4\] macrocyclic tetrapods](#),

M.E. Briggs, K.E. Jelfs, S.Y. Chong, C. Lester, M. Schmidtman, D.J. Adams and A.I. Cooper,
Cryst. Growth Des. (2013); DOI: 10.1021/cg401171v

[5] [Predicted crystal energy landscapes of porous organic cages](#),

E.O. Pyzer-Knapp, H.P.G. Thompson, F. Schiffmann, K.E. Jelfs, S.Y. Chong, M.A. Little, A.I. Cooper and G.M. Day,
Chemical Science (2014), 5, 2235-2245; DOI: 10.1039/C4SC00095A

[6] [Which conformations make stable crystal structures? Mapping crystalline molecular geometries to the conformational energy landscape](#),

H.P.G. Thompson and G.M. Day,
Chemical Science (2014), 5, 3173-3182; DOI: 10.1039/C4SC01132E

*[7] [Controlling the crystallization of porous organic cages: molecular analogs of isoreticular frameworks using shape-specific directing solvents](#),

T. Hasell, J.L. Culshaw, S.Y. Chong, M. Schmidtman, M.A. Little, K.E. Jelfs, E.O. Pyzer-Knapp, H. Shepherd, D.J. Adams, G.M. Day, and A.I. Cooper,
Journal of the American Chemical Society (2014) 136, 1438-1448; DOI: 10.1021/ja409594s

From Nora De Leeuw's Group

[1] [The onset of calcium carbonate nucleation: a computational study](#),

D. Di Tommaso and N.H. de Leeuw,
Geochim. Cosmochim. Acta (2008) 72, A219

[2] The onset of calcium carbonate nucleation: a density functional theory molecular dynamics and hybrid microsolvation/continuum study,
D. Di Tommaso and N.H. de Leeuw,
J. Phys. Chem. B (2008) 112, 6965–6975; DOI: 10.1021/jp801070b

[3] Hydrogen transfer and microhydration properties of $H_nPO_4^{3-n}$ ($n = 0-3$) in water studied by first principles molecular dynamics simulations,
E. Tang, D. Di Tommaso and N.H. de Leeuw,
J. Chem. Phys. (2009) 130, 234502-234511; DOI: 10.1063/1.3143952

[4] $MeHCO_3^+$ and $MeCO_3$ ($Me = Ca$ and Mg) species in aqueous solution: insights from quantum mechanical calculations,
D. Di Tommaso and N.H. de Leeuw,
Geochim. Cosmochim. Acta (2009) 73, A294

[5] Theoretical study of the dimerization of calcium carbonate in aqueous solution under natural water conditions,
D. Di Tommaso and N. H. de Leeuw,
Geochim. Cosmochim. Acta (2009) 73, 5394-5405; DOI: 10.1016/j.gca.2009.06.003

[6] Structure and dynamics of the hydrated magnesium ion and solvated magnesium carbonates: Insights from first principles simulations,
D. Di Tommaso and N.H. de Leeuw,
Phys. Chem. Chem. Phys. (2010) 12, 894-901; DOI: 10.1039/b915329b

[7] Modelling the nucleation of metal carbonates from aqueous solution: the importance of the hydration shell in the monomer formation,
D. Di Tommaso and N. H. de Leeuw,
Geochim. Cosmochim. Acta (2010) 74, A236

[8] Effect of phosphonates on calcite-solution reactions,
E. Ruiz-Agudo, C.V. Putnis, D. Di Tommaso, N.H. de Leeuw and A. Putnis,
Geochim. Cosmochim. Acta (2010) 74, A891

[9] Interactions between organophosphonate-bearing solutions and {1014} calcite surfaces. An AFM and Car-Parrinello molecular dynamics study,
E. Ruiz-Agudo, D. Di Tommaso, C.V. Putnis, N.H. de Leeuw and A. Putnis,
Cryst. Growth Des. (2010) 10, 3022–3035; DOI: 10.1021/cg1000864

[10] An ab initio molecular dynamics study of bioactive phosphate glasses,
E. Tang, D. Di Tommaso and N.H. de Leeuw,
Advanced Engineering Materials (Special Section: Euromat 2009 – Materials for Healthcare) (2010) 12, B331-B338

[11] First principles simulations of the structural and dynamical properties of hydrated metal ions Me^{2+} and solvated metal carbonates ($Me = Ca, Mg$ and Sr),
D. Di Tommaso and N.H. de Leeuw,
Cryst. Growth Des. (2010) 10, 4292–4302; DOI: 10.1021/cg100055p

[12] Accuracy of microsolvation-continuum approaches in the calculation of pKa and free energy of formation of phosphates in aqueous solution,
E. Tang, D. Di Tommaso and N.H. de Leeuw,
Phys. Chem. Chem. Phys. (2010) 12, 13804–13815; DOI: 10.1039/c0cp00175a

[13] A density functional theory study of structural, mechanical and electronic properties of crystalline phosphorus pentoxide,
R. I. Ainsworth, D. Di Tommaso and N.H. de Leeuw,
J. Chem. Phys. (2011) 135, 234513; DOI: 10.1063/1.3666017

[14] Polarizable force field development and molecular dynamics study of phosphate-based glasses,
R.I. Ainsworth, D. Di Tommaso, J.K. Christie and N.H. de Leeuw,
J. Chem. Phys. (2012) 137, 234502; DOI: 10.1063/1.4770295

[15] Density functional theory and interatomic potential study of structural, mechanical and surface properties of calcium oxalate materials,
D. Di Tommaso, S.E. Ruiz Hernández, Z. Du and N.H. de Leeuw,
RSC Adv. (2012) 2, 4664–4674; DOI: 10.1039/c2ra00832g

[16] Calcite surface structure and reactivity: molecular dynamics simulations and macroscopic surface modelling of the calcite–water interface,
M. Wolthers, D. Di Tommaso, Z. Dub and N.H. de Leeuw,
Phys. Chem. Chem. Phys. (2012) 14, 15145–15157; DOI: 10.1039/c2cp42290e

- [17] Cation distribution and mixing thermodynamics in Fe/Ni thiospinels, S. Haider, R. Grau-Crespo, A.J. Devey and N.H. de Leeuw, *Geochim. Cosmochim. Acta* (2012) 88, 275-282; DOI: 10.1016/j.gca.2012.04.007
- [18] Nanoscale chains control the solubility of phosphate glasses for biomedical applications, J.K. Christie, R.I. Ainsworth, D. Di Tommaso and N.H. de Leeuw, *J. Phys. Chem. B* (2013) 117, 10652–10657; DOI: 10.1021/jp4058115
- [19] A comparative DFT study of the mechanical and electronic properties of greigite Fe₃S₄ and magnetite Fe₃O₄, A. Roldan, D. Santos-Carballal and N.H. de Leeuw, *J. Chem. Phys.* (2013) 138, 204712; DOI: 10.1063/1.4807614
- [20] The role of hydrogen bonding and proton transfer in the formation of uracil networks on the gold (100) surface: a density functional theory approach, S. Irrera, A. Roldan, G. Portalone and N.H. de Leeuw, *J. Phys. Chem. C* (2013) 117, 3949–3957; DOI: 10.1021/jp3094353
- [21] Density functional theory simulations of the structure, stability and dynamics of iron sulphide clusters in water, S. Haider, D. Di Tommaso and N.H. de Leeuw, *Phys. Chem. Chem. Phys.* (2013) 15, 4310-4319; DOI: 10.1039/C3CP43560A
- [22] Adsorption of methylamine on mackinawite (FES) surfaces: a density functional theory study, N.Y. Dzade, A. Roldan and N.H. de Leeuw, *J. Chem. Phys.* (2013) 139, 124708; DOI: 10.1063/1.4822040
- [23] Variations in calcite growth kinetics with surface topography: molecular dynamics simulations and process-based growth kinetics modelling, M. Wolthers, D. Di Tommaso, Z. Du and N.H. de Leeuw, *Cryst. Eng. Comm.* (2013) 15, 5506–5514; DOI: 10.1039/c3ce40249e
- [24] Modelling the structural evolution of ternary phosphate glasses from melts to solid amorphous materials, D. Di Tommaso, R.I. Ainsworth, E. Tang and N.H. de Leeuw, *J. Mater. Chem. B* (2013) 1, 5054–5066; DOI: 10.1039/c3tb20662a
- [25] Adsorption of hydrazine on the perfect and defective copper (111) surface: A dispersion-corrected DFT study, S.S. Tafreshi, A. Roldan, N.Y. Dzade and N.H. de Leeuw, *Surf. Sci.* (2014) 622, 1–8; DOI: 10.1016/j.susc.2013.11.013
- [26] The surface chemistry of NO_x on mackinawite (FeS) surfaces: A DFT-D2 study, N.Y. Dzade, A. Roldan and N.H. de Leeuw, *Phys. Chem. Chem. Phys.* (2014) 16, 15444–15456; DOI: 10.1039/c4cp01138d
- [27] A density functional theory study of the adsorption of benzene on Hematite (α-Fe₂O₃) surfaces, N.Y. Dzade, A. Roldan and N.H. de Leeuw, *Minerals* (2014) 4, 89–115; DOI: 10.3390/min4010089
- *[28] A DFT study of the structures, stabilities and redox behaviour of the major surfaces of magnetite Fe₃O₄, D. Santos-Carballal, A. Roldan, R. Grau-Crespo and N.H. de Leeuw, *Phys. Chem. Chem. Phys.* (2014) 16, 21082–21097. DOI: 10.1039/c4cp00529e
- *[29] Density functional theory study of the adsorption of hydrazine on the perfect and defective copper (100), (110), and (111) surfaces, S.S. Tafreshi, A. Roldan, and N.H. de Leeuw, *J. Phys. Chem. C* (2014) 118 (45), 26103–26114; DOI: 10.1021/jp5078664

From Devis DiTommaso's Group

- [1] The molecular self-association of carboxylic acids in solution: testing the validity of the link hypothesis using a quantum mechanical continuum solvation approach, D. Di Tommaso, *Cryst. Eng. Comm.* (2013) 15, 5506–5514; DOI: 10.1039/c3ce40539g
- [2] Modelling the effects of salt solutions on the hydration of calcium ions, D. Di Tommaso, E. Ruiz-Agudo, N.H. de Leeuw, A. Putnis and C.V. Putnis, *Phys. Chem. Chem. Phys.* (2014) 16, 7772–7785; DOI: 10.1039/c3cp54923b
- *[3] Density Functional Theory Study of the Oligomerization of Carboxylic Acids, D. Di Tommaso and K.L. Watson, *J. Phys. Chem. A* (2014) 118, 11098–11113; DOI: 10.1021/jp509100u

From Dorothy Duffy's Group

[1] Including the effects of electronic stopping and electron-ion interactions in radiation damage simulations,

D.M. Duffy and A.M. Rutherford,
J. Phys.: Condens. Matter (2007) 19, 016207; DOI: 10.1088/0953-8984/19/1/016207

[2] The effect of electron-ion interactions on radiation damage simulations,

A.M. Rutherford and D.M. Duffy,
J. Phys.: Condens. Matter (2007) 19, 496201; DOI: 10.1088/0953-8984/19/49/496201

[3] Making tracks in metals,

D.M. Duffy, N. Itoh, A.M. Rutherford and A.M. Stoneham,
J. Phys.: Condens. Matter (2009) 21, 474205; DOI: 10.1088/0953-8984/20/8/082201

[4] An ab initio study of the effect of charge localization on oxygen defect formation and migration energies in MgO,

J. Mulroue and D.M. Duffy,
Proc. Roy. Soc. A (2011) 467, 2054; DOI: 10.1098/rspa.2010.0517

[5] Trapping of He in intrinsic defects in zirconolite,

J. Mulroue, M. Watkins, A.J. Morris and D.M. Duffy,
J. Nucl. Mater. (2013) 437 261–266; DOI: 10.1016/j.jnucmat.2013.02.037

[6] Charge localization on the hexa-interstitial cluster in MgO,

J. Mulroue, B.P. Uberuaga and D.M. Duffy,
J. Phys. Condens. Matter (2013) 25, 065502; DOI: 10.1088/0953-8984/25/6/065502

From Martin Dove's Group

[1] Simulation study of pressure and temperature dependence of the negative thermal expansion in Zn(CN)₂,

H. Fang, M.T. Dove, L.H.N. Rimmer, and A.J. Misquitta
Phys. Rev. B (2013) 88, 104306; DOI: 10.1103/PhysRevB.88.104306

[2] Pressure-induced softening as a common feature of framework structures with negative thermal expansion,

H. Fang and M.T. Dove
Phys. Rev. B (2013) 87, 214109; DOI: 10.1103/PhysRevB.87.214109

[3] Framework flexibility and the negative thermal expansion mechanism of copper(I) oxide Cu₂O,

L.H.N. Rimmer, M.T. Dove, B. Winkler, D.J. Wilson, K. Refson and A.L. Goodwin
Phys. Rev. B (2014) 89, 214115, 1-10; DOI: 10.1103/PhysRevB.89.214115

*[4] Acoustic phonons and negative thermal expansion in MOF-5,

L.H.N. Rimmer, M.T. Dove, A.L. Goodwin and D.C. Palmer
Phys. Chem. Chem. Phys. (2014) 16, 21144–21152, DOI: 10.1039/c4cp01701c

*[5] Ag-Ag dispersive interaction and physical properties of Ag₃Co(CN)₆,

H. Fang, M.T. Dove and K. Refson
Physical Review B (2014) 90, 054302, DOI: 10.1103/PhysRevB.90.054302

*[6] Structural changes in zirconolite under alpha-decay,

H.F. Chappell, M.T. Dove, K. Trachenko, R.E.A. McKnight, M.A. Carpenter and S.A.T. Redfern
Journal of Physics: Condensed Matter (2013) 25, 055401, DOI: 10.1088/0953-8984/25/5/055401

*[7] A phenomenological expression to describe the temperature dependence of pressure-induced softening in negative thermal expansion materials,

H. Fang and M.T. Dove
Journal of Physics: Condensed Matter (2014) 26, 115402, DOI: 10.1088/0953-8984/26/11/115402

From Paul Elliott's Group

[1] Unambiguous characterisation of a photoreactive ligand loss intermediate,

C.E. Welby, C.R. Rice and P.I.P. Elliott
Angew. Chem. Int. Ed. (2013) 52, 10826-10829; DOI: 10.1002/anie.201304219

[2] Luminescent biscyclometalated arylpyridine iridium(III) complexes with 4,4'-bi-1,2,3-triazolyl ancillary ligands,

C.E. Welby, L. Gilmartin, R.R. Marriott, A. Zahid, C.R. Rice, E.A. Gibson and P.I.P. Elliott
Dalton Trans. (2013) 42, 13527- 13536; DOI: 10.1039/C3DT51284C

Novel triphenylamine-modified ruthenium(II) terpyridine complexes for nickel oxide-based cathodic dye-sensitized solar cells,

[3] C.J. Wood, K.C.D. Robson, P.I.P. Elliott, C.P. Berlinguette and E.A. Gibson
RSC Adv. (2013) 4, 5782-5791; DOI: 10.1039/c3ra44690e

From Matthew Foulkes's Group

[1] [On the growth of Al₂O₃ scales,](#)

A. H. Heuer, T. Nakagawa, M.Z. Azar, D.B. Hovis, J.L. Smialek, B. Gleeson, N.D.M. Hine, H. Guhl, H.-S. Lee, P. Tangney, W.M.C. Foulkes and M.W. Finnis

Acta Mater. (2013) 61, 6670–6683; DOI: 10.1016/j.actamat.2013.07.024

From Ricardo Grau-Crespo's Group

[1] [Electronic structure and magnetic coupling in FeSbO₄: A DFT study using hybrid functional and GGA+U methods,](#)

R. Grau-Crespo, F. Corà, A.A. Sokol, N.H. de Leeuw and C.R.A. Catlow,
Phys. Rev. B (2006) 73, 035116; DOI: 10.1103/PhysRevB.73.035116

[2] [The effect of cation coordination on the properties of oxygen vacancies in FeSbO₄,](#)

R. Grau-Crespo, I.P.R. Moreira, F. Illas, N.H. de Leeuw and C.R.A. Catlow,
J. Mater. Chem. (2006) 16, 1943–1949; DOI: 10.1039/b518219k

[3] [A computer modeling study of redox processes on the FeSbO₄ \(100\) surface,](#)

R. Grau-Crespo, C.R.A. Catlow and N.H. de Leeuw,
Journal of Catalysis (2007) 248, 77–88; DOI: 10.1016/j.jcat.2007.02.015

[4] [Symmetry-adapted configurational modelling of fractional site occupancy in solids,](#)

R. Grau-Crespo, S. Hamad, C.R.A. Catlow and N.H. de Leeuw,
J. Phys.: Condens. Matter (2007) 19, 256201; DOI: 10.1088/0953-8984/19/25/256201

[5] [Electronic charge transfer between ceria surfaces and gold adatoms: a GGA+U investigation,](#)

N.C. Hernandez, R. Grau-Crespo, N.H. de Leeuw and J.F. Sanz,
Phys. Chem. Chem. Phys. (2009) 11, 5246–5252; DOI: 10.1039/b820373c

[6] [Redox properties of gold-substituted zirconia surfaces,](#)

R. Grau-Crespo, N.C. Hernandez, J.F. Sanz and N.H. de Leeuw,
J. Mater. Chem. (2009) 19, 710–717; DOI: 10.1039/b812245h

[7] [Thermodynamics of hydrogen vacancies in MgH₂ from first-principles calculations and grand-canonical statistical mechanics,](#)

R. Grau-Crespo, K.C. Smith, T.S. Fisher, N.H. de Leeuw and U.V. Waghmare,
Phys. Rev. B (2009) 80, 174117; DOI: 10.1103/PhysRevB.80.174117

[8] [Electronic and magnetic structure of Fe₃S₄: GGA+U investigation,](#)

A.J. Devey, R. Grau-Crespo and N.H. de Leeuw,
Phys. Rev. B (2009) 79, 195126; DOI: 10.1103/PhysRevB.79.195126

[9] [On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO₂\(111\),](#)

M.M. Branda, N.J. Castellani, R. Grau-Crespo, N.H. de Leeuw, N.C. Hernandez, J.F. Sanz, K.M. Neyman and F. Illas,
J. Chem. Phys. (2009) 131, 094702; DOI: 10.1063/1.3216102

[10] [Vacancy ordering and electronic structure of gamma-Fe₂O₃ \(maghemite\): a theoretical investigation,](#)

R. Grau-Crespo, A.Y. Al-Baitai, I. Saadoun and N.H. De Leeuw,
J. Phys. – Cond. Matter (2010) 22, 255401; DOI: 10.1088/0953-8984/22/25/255401

[11] [Electronic structure and redox properties of the Ti-doped zirconia \(111\) surface,](#)

H.R. Chauke, P. Murovhi, P.E. Ngoepe, N.H. de Leeuw and R. Grau-Crespo,
J. Phys. Chem. C (2010) 114, 15403-15409; DOI: 10.1021/jp103181q

[12] [Dopant-vacancy binding effects in Li-doped magnesium hydride,](#)

K.C. Smith, T.S. Fisher, U.V. Waghmare and R. Grau-Crespo,
Phys. Rev. B (2010) 82, 134109; DOI: 10.1103/PhysRevB.82.134109

[13] [Phase separation and surface segregation in ceria-zirconia solid solutions,](#)

R. Grau-Crespo, N.H. de Leeuw, S. Hamad and U.V. Waghmare,
Proc. Royal Soc. A (2011) 467, 1925-1938; DOI: 10.1098/rspa.2010.0512

[14] [The interplay between dopants and oxygen vacancies in the magnetism of V-doped TiO₂,](#)

R. Grau-Crespo and U. Schwingenschlögl,
J. Phys.: Condens. Matter (2011) 23, 334216; DOI: 10.1088/0953-8984/23/33

[15] [Band gap control via tuning of inversion degree in CdIn₂S₄,](#)

Y. Seminovski, P. Palacios, P. Wahnón and R. Grau-Crespo,
Appl. Phys. Lett. (2012) 100, 102112; DOI: 10.1063/1.3692780

[16] [A density functional theory study of rutile VO₂ surfaces,](#)

T.A. Mellan and R. Grau-Crespo,

J. Chem. Phys. (2012) 137, 154706; DOI: 10.1063/1.4758319

[17] [Why the Heyd-Scuseria-Ernzerhof hybrid functional description of VO₂ phases is not correct,](#)

R. Grau-Crespo, H. Wang and U. Schwingenschlöggl,
Phys. Rev. B (2012) 86, 081101(R); DOI: 10.1103/PhysRevB.86.081101

[18] [Lithium and oxygen adsorption at the β-MnO₂ \(110\) surface,](#)

T.A. Mellan, K. Maenetja, P.E. Ngoepe, S.M. Woodley, C.R.A. Catlow and R. Grau-Crespo,
J. Mater. Chem. A (2013); DOI: 10.1039/c3ta13559d

[19] [Spin polarization, orbital occupation and band gap opening in vanadium dioxide: the effect of screened Hartree–Fock exchange,](#)

H. Wang, T.A. Mellan, R. Grau-Crespo and U. Schwingenschlöggl,
Chem. Phys. Lett. (2014), 608, 126-129; DOI: 10.1016/j.cplett.2014.05.070

From Clare Grey's Group

[1] [Structural modulation in the high capacity battery cathode material LiFeBO₃,](#)

Y. Janssen, D.S. Middlemiss, S.-H. Bo, C.P. Grey and P.G. Khalifah
J. Am. Chem. Soc. (2012) 134, 12516; DOI: 10.1021/ja301881c

[2] [Probing cation and vacancy ordering in the perovskite BaSn_{1-x}Y_xO_{3-δ} electrolyte by NMR spectroscopy and first principles calculations: Implications for proton mobility,](#)

L. Buannic, F. Blanc, D.S. Middlemiss and C.P. Grey
J. Am. Chem. Soc. (2012) 134, 12516; DOI: 10.1021/ja304712v

[3] [Spin-transfer pathways in paramagnetic lithium transition metal phosphates from combined broadband isotropic solid-state MAS NMR spectroscopy and DFT calculations,](#)

R.J. Clément, A.J. Pell, D.S. Middlemiss, F.C. Strobridge, B.X.Y. Zhu, J.K. Miller, M.S. Whittingham, L. Emsley, C.P. Grey and G. Pintacuda

J. Am. Chem. Soc. (2012) 134, 17178-17185; DOI: 10.1021/ja306876u

[4] [Density functional theory-based bond pathway decompositions of hyperfine shifts: equipping solid-state NMR to characterize atomic environments in paramagnetic materials,](#)

D.S. Middlemiss, A.J. Iltott, R.J. Clément, F.C. Strobridge and C.P. Grey
Chem. Mat. (2013) 25, 9, 1723–1734; DOI: 10.1021/cm400201t

From John Harding's Group

[1] [Computational techniques at the organic-inorganic interface in biomineralization,](#)

J.H. Harding, D.M. Duffy, M.L. Sushko, P.M. Rodger, D. Quigley and J.A. Elliott
Chem. Rev. (2008) 108, 4823-4854; DOI: 10.1021/cr078278y

[2] [A demonstration of the inhomogeneity of the local dielectric response of proteins by molecular dynamics simulations,](#)

G.N. Patargias, S.A. Harris and J.H. Harding
J. Chem. Phys. (2010) 132, 235103; DOI: 10.1063/1.3430628

[3] [Charge disproportionation and Jahn-Teller distortion in LiNiO₂ and NaNiO₂: A density functional theory study,](#)

H. Chen, C.L. Freeman and J.H. Harding
Phys. Rev. B (2011) 84, 085108; DOI: 10.1103/PhysRevB.84.085108

[4] [Nature of the hole states in Li-doped NiO,](#)

H. Chen and J.H. Harding
Phys. Rev. B (2012) 85, 115127; DOI: 10.1103/PhysRevB.85.115127

[5] [Atomistic simulation of doping effects on growth and charge transport in Si/Ag interfaces in high-performance solar cells,](#)

K.T. Butler, J.H. Harding
Phys. Rev. B (2012) 86, 245319; DOI: 10.1103/PhysRevB.86.245319

[6] [Stoichiometrically graded SiNx for improved surface passivation in high performance solar cells,](#)

K.T. Butler, J.H. Harding, M.P.W.E. Lamers and A.W. Weeber
J. Appl. Phys. (2012) 85, 112, 094303; DOI: 10.1063/1.4764012

[7] [Effects of cationic substitution on structural defects in layered cathode materials LiNiO₂,](#)

H.R. Chen, J.A. Dawson and J.H. Harding
J. Mater. Chem. A (2014) 2, 7988-7996; DOI: 10.1039/c4ta00637b

*[8] [Entropy of molecular binding at solvated mineral surfaces,](#)

C.L. Freeman and J.H. Harding,
Journal of Physical Chemistry C (2014) 118, 1506-1514; DOI: 10.1021/jp407122u

From Nicholas Harrison's Group

- [1] Density functional study of the magnetic coupling in $V(\text{TCNE})_2$, G.C. De Fusco, L. Pisani, B. Montanari and N.M. Harrison, *Phys. Rev. B* (2009) 79, 085201; DOI: 10.1103/PhysRevB.79.085201
- [2] Structure and stability of alpha- AlF_3 surfaces, C. L. Bailey, S. Mukhopadhyay, A. Wander, B.G. Searle and N. M. Harrison, *J Phys. Chem. C* (2009) 113, 4976; DOI: 10.1021/jp810719h
- [3] Reactivity of the beta- $\text{AlF}_3(100)$ surface: defects, fluorine mobility and catalysis of the CCl_2F_2 dismutation reaction, C. L. Bailey, S. Mukhopadhyay, A. Wander, B.G. Searle, J.M. Carr and N. M. Harrison, *Phys. Chem. Chem. Phys.* (2010) 12, 6124; DOI: 10.1039/b920542j
- [4] Defect physics of CuGaS_2 , C.L. Bailey, L. Liborio, G. Mallia, S. Tomic and N.M. Harrison, *Phys. Rev. B* (2010) 81, 205214; DOI: 10.1103/PhysRevB.81.205214
- [5] Half-metallicity in the ferrimagnet $\text{Nb}(\text{TCNE})_2$ from first principles, G.C. De Fusco, B. Montanari and N.M. Harrison, *Phys. Rev. B* (2010) 82, 220404; DOI: 10.1103/PhysRevB.82.220404
- [6] Periodic quantum mechanical simulation of the He- $\text{MgO}(100)$ interaction potential, R. Martinez-Casado, G. Mallia, D. Usvyat, L. Maschio, S. Casassa, M. Schuetz and N.M. Harrison, *J. Chem. Phys.* (2011) 134, 014706; DOI: 10.1063/1.3517868
- [7] Chemistry of defect induced photoluminescence in chalcopyrites: The case of CuAlS_2 , L. M. Liborio, C. L. Bailey, G. Mallia, S. Tomic and N. M. Harrison, *J. Appl. Phys.* (2011) 109, 023519; DOI: 10.1063/1.3544206
- [8] An efficient method for computing the binding energy of an adsorbed molecule within a periodic approach. The application to vinyl fluoride at rutile $\text{TiO}_2(110)$ surface, J. Scaranto, G. Mallia and N.M. Harrison, *Comp. Mat. Sci.* (2011) 50, 2080; DOI: 10.1016/j.commatsci.2011.02.011
- [9] An alternative approach for the calculation of correlation energy in periodic systems: a hybrid MP2(B3LYP) study of the He- $\text{MgO}(100)$ interaction, R. Martinez-Casado, G. Mallia and N.M. Harrison, *Chem. Commun.* (2011) 47, 4385; DOI: 10.1039/C0CC05541G
- [10] Parallel implementation of the ab initio CRYSTAL program: Electronic structure calculations for periodic systems, I.J. Bush, S. Tomic, B.G. Searle, G. Mallia, C.L. Bailey, B. Montanari, L. Bernasconi, J.M. Carr and N.M. Harrison, *Proc. R. Soc. A* (2011) 467, 2112; DOI: 10.1098/rspa.2010.0563
- [11] A hybrid density functional study of water adsorption on rutile $\text{TiO}_2(110)$ for applications in solar hydrogen production, M. Patel, G. Mallia, L. Liborio and N.M. Harrison, NSTI, Nanotech2011 Technical Proceedings, TechConnect World 2011, June 13-16 2011, Boston, MA
- [12] He-atom scattering from $\text{MgO}(100)$: calculating diffraction peak intensities from first principles, R. Martinez-Casado, G. Mallia, D. Usvyat, L. Maschio, S. Casassa, M. Schuetz and N.M. Harrison, *Phys. Chem. Chem. Phys.* (2011) 13, 14750; DOI: 10.1039/C1CP21212E
- [13] Thermodynamic stability of LaMnO_3 and its competing oxides: A hybrid density functional study of an alkaline fuel cell catalyst, E.A. Ahmad, L. Liborio, D. Kramer, G. Mallia, A.R. Kucernak and N.M. Harrison, *Phys. Rev. B* (2011) 84, 085137; DOI: 10.1103/PhysRevB.84.085137
- [14] Ab initio calculation of the $\text{MgO}(100)$ interaction with He and Ne: a HF+MP2 and HF+MP2(B3LYP) comparison, R. Martinez-Casado, G. Mallia and N. M. Harrison, *Chem. Commun.*, (2011) 47, 11630; DOI: 10.1039/C1CC14623H
- [15] Atomic structure of the (001) surface of CuGaSe_2 , L. Liborio, S. C. Chew and N. M. Harrison, *Surf. Sci.* (2012) 606, 496; DOI: 10.1016/j.susc.2011.11.018
- [16] Ab initio complex band structure of conjugated polymers: Effects of hybrid density functional theory and GW schemes, A. Ferretti, G. Mallia, L. Martin-Samos, G. Bussi, A. Ruini, B. Montanari and N.M. Harrison, *Phys. Rev. B* (2012) 85, 235105; DOI: 10.1103/PhysRevB.85.235105
- [17] Comment on "2D Atomic Mapping of Oxidation States in Transition Metal Oxides by Scanning Transmission Electron Microscopy and Electron Energy-Loss Spectroscopy"

- E. A. Ahmad, G. Mallia, D. Kramer, V. Tileli, A. R. Kucernak, and N. M. Harrison
Phys. Rev. Lett., (2012) 108, 259701; DOI: 10.1103/PhysRevLett.108.259701
- [18] Water adsorption on rutile TiO₂(110) for applications in solar hydrogen production: A systematic hybrid-exchange density functional study,
 M. Patel, G. Mallia, L. Liborio and N.M. Harrison,
Phys. Rev. B (2012) 86, 045302; DOI: 10.1103/PhysRevB.86.045302
- [19] A quantum-mechanical study of the adsorption of prototype dye molecules on rutile-TiO₂(110): a comparison between catechol and isonicotinic acid,
 F. Risplendi, G. Cicero, G. Mallia and N.M. Harrison,
Phys. Chem. Chem. Phys. (2013) 15, 235; DOI: 10.1039/C2CP42078C
- [20] A hybrid-exchange density functional study of Ca-doped LaMnO₃,
 R. Korotana, G. Mallia, Z. GerCSI, and N.M. Harrison,
J. Appl. Phys. (2013) 113, 17A910; DOI: 10.1063/1.4794877
- [21] Simulating constant current STM images of the rutile TiO₂ (110) surface for applications in solar water splitting,
 F.F. Sanches, G. Mallia and N.M. Harrison,
MRS Proceedings (2013), 1494, mrsf12-1494-f02-02; DOI: 10.1557/opl.2013.236
- [22] The structure of water on rutile TiO₂(110) for applications in solar hydrogen production: towards a predictive model using hybrid-exchange density functional theory,
 M. Patel, G. Mallia and N.M. Harrison,
MRS Proceedings (2013), 1542, mrss13-1542-g10-03; DOI: 10.1557/opl.2013.628
- [23] The stability of LaMnO₃ surfaces: a hybrid exchange density functional theory study of an alkaline fuel cell catalyst,
 E.A. Ahmad, G. Mallia, D. Kramer, A.R. Kucernak and N.M. Harrison,
J. Mater. Chem. A (2013) 1, 11152; DOI: 10.1039/C3TA11382E

From Saiful Islam's Group

- [1] Li₂MnSiO₄ lithium battery material: atomic-scale study of defects, lithium mobility, and trivalent dopants,
 N. Kuganathan and M.S. Islam,
Chem. Mater. (2009) 21, 5196-5202; DOI: 10.1021/cm902163k
- [2] Lithium insertion and transport in the TiO₂-B anode material: A computational study,
 C. Arrouvel, S.C. Parker and M.S. Islam,
Chem. Mater. (2009) 21, 4778-4783; DOI: 10.1021/cm900373u
- [3] Solid-state materials for clean energy: Insights from atomic scale modeling,
 M.S. Islam and P.R. Slater,
MRS Bulletin (2009) 34, 935-941; DOI: 10.1557/mrs2009.216
- [4] Lithium coordination sites in Li_xTiO₂(B): A structural and computational study,
 A.R. Armstrong, C. Arrouvel, V. Gentili, S.C. Parker, M.S. Islam and P.G. Bruce,
Chem. Mater. (2010) 22, 6426-6432; DOI: 10.1021/cm102589x
- [5] Recent atomistic modelling studies of energy materials: batteries included,
 M.S. Islam,
Phil. Trans. R. Soc. A (2010) 368, 3255-3267; DOI: 10.1098/rsta.2010.0070
- [6] Protonic defects and water incorporation in Si and Ge-based apatite ionic conductors,
 P.M. Panchmatia, A. Orera, E. Kendrick, J.V. Hanna, M.E. Smith, R.R. Slater and M.S. Islam,
J. Mater. Chem. (2010) 20, 2766-2772; DOI: 10.1039/B924220A
- [7] Anti-site defects and ion migration in the LiFe_{0.5}Mn_{0.5}PO₄ mixed-metal cathode material,
 G.R. Gardiner and M.S. Islam,
Chem. Mater. (2010) 22, 1242-1248; DOI: 10.1021/cm902720z
- [8] The lithium intercalation process in the low voltage lithium battery anode Li_{1+x}V_{1-x}O₂,
 A.R. Armstrong, C. Lyness, P. Panchmatia, M.S. Islam and P.G. Bruce,
Nature Materials (2011) 10, 223-229; DOI: 10.1038/NMAT2967
- [9] Structure and lithium transport pathways in Li₂FeSiO₄ cathodes for lithium batteries,
 A.R. Armstrong, N. Kuganathan, M.S. Islam and P.G. Bruce,
J. Am. Chem. Soc. (2011) 133, 13031-13035; DOI: 10.1021/ja2018543
- [10] Elucidation of oxygen defects and novel transport mechanisms in apatite ionic conductors: combined 17O NMR and modeling studies,
 P.M. Panchmatia, A. Orera, G.J. Rees, M.E. Smith, J. Hanna, P.R. Slater and M.S. Islam,
Angew. Chemie. (2011) 50, 9328-9333; DOI: 10.1002/anie.201102064

- [11] Structural and electronic properties of CuSbS_2 and CuBiS_2 : potential absorber materials for thin-film solar cells, J.T.R. Dufton, A. Walsh, P.M. Panchmatia, L.M. Peter, D. Colombara and M.S. Islam, *Phys. Chem. Chem. Phys.* (2012) 14, 7229-7233; DOI: 10.1039/c2cp40916j
- [12] Water adsorption and its effect on the stability of low index stoichiometric and reduced surfaces of ceria, M. Molinari, S.C. Parker, D.C. Sayle, and M.S. Islam, *J. Phys. Chem. C.* (2012) 116, 7073-7082; DOI: 10.1021/jp300576b
- [13] Insights into changes in voltage and structure of $\text{Li}_2\text{FeSiO}_4$ polymorphs for lithium-ion batteries, C. Eames, A.R. Armstrong, P.G. Bruce and M.S. Islam, *Chem. Mater.* (2012) 24, 2155-2161; DOI: 10.1021/cm300749w
- [14] Importance of anisotropic Coulomb interactions and exchange to the band gap and antiferromagnetism of $\beta\text{-MnO}_2$ from DFT+U, D.A. Tompsett, D.S. Middlemiss and M.S. Islam, *Phys. Rev. B* (2012) 86, 205126; DOI: 10.1103/PhysRevB.86.205126
- [15] Nanostructuring of $\beta\text{-MnO}_2$: the important role of surface to bulk ion migration, D.A. Tompsett, S.C. Parker, P.G. Bruce and M.S. Islam, *Chem. Mater.* (2013) 25, 536; DOI: 10.1021/cm303295f
- [16] Defect chemistry and lithium-ion migration in polymorphs of the cathode material $\text{Li}_2\text{MnSiO}_4$, C.A.J. Fisher, N. Kuganathan and M.S. Islam, *J. Mater. Chem. A.* (2013) 1, 4207-4214; DOI: 10.1039/c3ta00111c
- [17] Defect and dopant properties of the alpha- and beta-polymorphs of the Li_3FeF_6 lithium battery material, E. Gonzalo, A. Kuhn, F. García-Alvarado and M.S. Islam, *J. Mater. Chem. A.* (2013) 1, 6588-6592; DOI: 10.1039/c3ta10630f
- [18] Electrochemistry of Hollandite $\alpha\text{-MnO}_2$: Li-ion and Na-ion insertion and Li_2O incorporation, D.A. Tompsett and M.S. Islam, *Chem. Mater.* (2013) 25, 2515-2526; DOI: 10.1021/cm400864n
- [19] Na-ion mobility in layered $\text{Na}_2\text{FePO}_4\text{F}$ and olivine $\text{Na}[\text{Fe},\text{Mn}]\text{PO}_4$, R. Tripathi, S.M. Wood, M.S. Islam and L.F. Nazar, *Energy Environ. Sci.* (2013) 6, 2257-2264; DOI: 10.1039/c3ee40914g
- [20] The shape of $\text{TiO}_2\text{-B}$ nanoparticles, Y.G. Andreev, P.M. Panchmatia, Z. Liu, S.C. Parker, M.S. Islam and P.G. Bruce, *J. Am. Chem. Soc.* (2014) 136, 6306-6312; DOI: 10.1021/ja412387c
- [21] Rutile (β -) MnO_2 surfaces and vacancy formation for high electrochemical and catalytic performance, D.A. Tompsett, S.C. Parker and M.S. Islam, *J. Am. Chem. Soc.* (2014) 136, 1418-1426; DOI: 10.1021/ja4092962
- [22] Lithium migration pathways and van der Waals effects in the LiFeSO_4OH battery material, C. Eames, J.M. Clark, G. Rouse, J.-M. Tarascon and M.S. Islam, *Chem. Mater.* (2014) 26, 3672-3678; DOI: 10.1021/cm5008203
- *[23] Sodium-ion battery cathodes $\text{Na}_2\text{FeP}_2\text{O}_7$ and $\text{Na}_2\text{MnP}_2\text{O}_7$: diffusion behaviour for high rate performance, J.M. Clark, P. Barpanda, A. Yamada and M.S. Islam, *J. Mater. Chem. A* (2014) 2, 11807-11812; DOI: 10.1039/C4TA02383H
- *[24] High voltage sulphate cathodes $\text{Li}_2\text{M}(\text{SO}_4)_2$ ($\text{M} = \text{Fe}, \text{Mn}, \text{Co}$): atomic-scale studies of lithium diffusion, surfaces and voltage trends, J.M. Clark, C. Eames, M. Reynaud, G. Rouse, J.N. Chotard, J.M. Tarascon and M.S. Islam, *J. Mater. Chem. A* (2014) 2, 7446-7453; DOI: 10.1039/C3TA15064J
- *[25] Rutile MnO_2 surfaces and vacancy formation for high electrochemical and catalytic performance, D.A. Tompsett, S.C. Parker and M.S. Islam, *J. Amer. Chem. Soc.* (2014) 136, 1418-1426; DOI: 10.1021/ja4092962
- *[26] Particle shapes and surface structures of olivine NaFePO_4 in comparison to LiFePO_4 , A. Whiteside, C.A.J. Fisher, S.C. Parker and M.S. Islam, *Phys. Chem. Chem. Phys.* (2014) 16, 21788-21794; DOI: 10.1039/C4CP02356K
- *[27] Surface Properties of $\alpha\text{-MnO}_2$: relevance to catalytic and supercapacitor behaviour, D.A. Tompsett, S.C. Parker and M.S. Islam, *J. Mater. Chem. A* (2014) 2, 15509-15518; DOI: 10.1039/C4TA00952E
- *[28] Lithium-ion diffusion mechanisms in the battery anode material $\text{Li}_{1+x}\text{V}_{1-x}\text{O}_2$,

P.M. Panchmatia, A.R. Armstrong, P.G. Bruce and M.S. Islam
Phys. Chem. Chem. Phys. (2014) 16, 21114-21118; DOI: 10.1039/C4CP01640H

*[29] [Ion intercalation into two-dimensional transition-metal carbides: global screening for new high capacity battery materials](#),

C. Eames and M.S. Islam
J. Am. Chem. Soc. (2014) 136, 16270-16276; DOI: 10.1021/ja508154e

From Kim Jelfs' Group

[1] [Controlling the crystallization of porous organic cages: molecular analogs of isorecticular frameworks using shape-specific directing solvents](#),

T. Hasell, J.L. Culshaw, S.Y. Chong, M. Schmidtman, M.A. Little, K.E. Jelfs, E.O. Pyzer-Knapp, H. Shepherd, D.J. Adams, G.M. Day and A.I. Cooper,
J. Am. Chem. Soc. (2014) 136, 1438-1448; DOI: 10.1021/ja409594s

From Roy Johnston's Group

[1] [Structures and stabilities of platinum-gold nanoclusters](#),

A.J. Logsdail, L.O. Paz-Borbon and R.L. Johnston
J. Comput. Theor. Nanosci. (2009) 6, 857-866; DOI: 10.1166/jctn.2009.1118

[2] [Chemisorption of CO and H on Pd, Pt and Au nanoclusters](#),

L.O. Paz-Borbón, R.L. Johnston, G. Barcaro and A. Fortunelli
Eur. Phys. J. D (2009) 52, 131-134; DOI: 10.1140/epjd/e2009-00041-9

[3] [Theoretical studies of palladium-gold nanoclusters: Pd-Au clusters with up to 50 atoms](#),

F. Pittaway, L.O. Paz-Borbón, R.L. Johnston, H. Arslan, R. Ferrando, C. Mottet, G. Barcaro and A. Fortunelli

J. Phys. Chem. C (2009) 113, 9141-9152; DOI: 10.1021/jp9006075

[4] [Investigation of the structures and chemical ordering of small Pd-Au clusters as a function of composition and potential parameterisation](#),

R. Ismail and R.L. Johnston

Phys. Chem. Chem. Phys. (2010) 12, 8607-8619; DOI: 10.1039/c004044d

[5] [Structure and chemical ordering of small Cu-Ag clusters](#)

S. Nunez and R.L. Johnston

J. Phys. Chem. C (2010) 114, 13255-13266; DOI: 10.1021/jp1048088

[6] [Theoretical and experimental studies of the optical properties of conjoined gold-palladium nanospheres](#),

A.J. Logsdail, N.J. Cookson, S.L. Horswell, Z.W. Wang, Z.Y. Li and R.L. Johnston

J. Phys. Chem. C (2010) 114, 21247-21251; DOI: 10.1021/jp108486a

[7] [The effect of CO and H chemisorption on the chemical ordering of bimetallic clusters](#),

P.S. West, R.L. Johnston, G. Barcaro and A. Fortunelli

J. Phys. Chem. C (2010) 114, 19678-19686; DOI: 10.1021/jp108387x

[8] [Energy landscape and global optimisation for a frustrated model protein](#),

M.T. Oakley, D.J. Wales and R.L. Johnston

J. Phys. Chem. B (2011) 115, 11525-11529; DOI: 10.1021/jp207246m

[9] [The effect of non-native interactions on the energy landscapes of frustrated model proteins](#),

M.T. Oakley, D.J. Wales and R.L. Johnston

J. Phys. Chem. B (2011) 115, 11525-11529; DOI: 10.1155/2012/192613

[10] [Dopant-induced 2D-3D transition in small Au-containing clusters: DFT-global optimisation of 8-atom Au-Ag nanoalloys](#),

S. Heiles, A.J. Logsdail, R. Schaefer and R.L. Johnston

Nanoscale (2012) 4, 1109-1115; DOI: 10.1039/C1NR11053E

[11] [Theoretical studies of Pt-Ti nanoparticles for potential use as PEMFC electrocatalysts](#),

P.C. Jennings, B.G. Pollet and R.L. Johnston

Phys. Chem. Chem. Phys. (2012) 14, 3134-3139; DOI: 10.1039/C2CP23430K

[12] [Development and optimisation of a novel genetic algorithm for identifying nanoclusters from scanning transmission electron microscopy images](#),

A.J. Logsdail, Z.Y. Li and R.L. Johnston

J. Comput. Chem. (2012) 33, 391-400; DOI: 10.1002/jcc.21976

[13] [Gas phase structures of bare Si₈ and Si₁₁ clusters from molecular beam electric deflection experiments](#),

D.A. Götz, S. Heiles, R.L. Johnston and R. Schaefer

J. Chem. Phys. (2012) 136, 186101; DOI: 10.1063/1.4717708

- [14] Interdependence of structure and chemical order in high symmetry (PdAu)_N nanoclusters, A.J. Logsdail and R.L. Johnston
RSC Adv. (2012) 2, 5863-5869; DOI: 10.1039/C2RA20309J
- [15] Nine-atom tin-bismuth clusters: mimicking excess electrons by element substitution, S. Heiles, K. Hofmann, R.L. Johnston and R. Schaefer
ChemPlusChem (2012) 77, 532-535; DOI: 10.1002/cplu.201200085
- [16] Bismuth-doped tin clusters: experimental and theoretical studies of neutral Zintl analogues, S. Heiles, R. L. Johnston and R. Schaefer
J. Phys. Chem. A (2012) 116, 7756-7764; DOI: 10.1021/jp304321u
- [17] Electronic properties of Pt-Ti nanoalloys and the effect on reactivity for use in PEMFCs, P.C. Jennings, B.G. Pollet and R.L. Johnston
J. Phys. Chem. C (2012) 116, 15241-15250; DOI: 10.1021/jp303577t
- [18] Predicting the optical properties of core-shell segregated and Janus Au-M nanoparticles (M = Ag, Pd), A.J. Logsdail and R.L. Johnston
J. Phys. Chem. C (2012) 116, 23616-23628; DOI: 10.1021/jp306000u
- [19] DFT study of the structures and energetics of 98-atom AuPd clusters, A. Bruma, R. Ismail, L.O. Paz-Borbon, H. Arslan, G. Barcaro, A. Fortunelli, Z.Y. Li and R.L. Johnston, *Nanoscale* (2013), 5, 646-652; DOI: 10.1039/C2NR32517A
- [20] Exploring the energy landscapes of cyclic tetrapeptides with discrete path sampling, M.T. Oakley and R.L. Johnston
J. Chem. Theory Comput. (2013), 9, 650-657; DOI: 10.1021/ct3005084
- [21] Theoretical study of the structures and chemical ordering of palladium-gold nanoalloys supported on MgO(100), R. Ismail, R. Ferrando and R.L. Johnston
J. Phys. Chem. C (2013) 117, 293-301; DOI: 10.1021/jp3093435
- [22] Symmetrisation schemes for global optimisation of atomic clusters, M.T. Oakley, R.L. Johnston and D.J. Wales
Phys. Chem. Chem. Phys. (2013) 15, 3965-3976; DOI: 10.1039/C3CP44332A
- [23] A density functional global optimisation study of neutral 8-atom Cu-Ag and Cu-Au clusters, C.J. Heard and R.L. Johnston
Europhys. J. D (2013) 67, 34; DOI: 10.1140/epjd/e2012-30601-7
- [24] A selective blocking method to control the overgrowth of Pt on Au nanorods, J. Fennell, D. He, A. Muche Tanyi, A.J. Logsdail, R.L. Johnston, Z.Y. Li and S.L. Horswell
J. Am. Chem. Soc. (2013) 135, 6554-6561; DOI: 10.1021/ja4003475
- [25] Faceting preferences for Au_N and Pd_N nanoclusters with high-symmetry motifs, A.J. Logsdail, Z.Y. Li and R.L. Johnston
Phys. Chem. Chem. Phys. (2013) 15, 8392-8400; DOI: 10.1039/C3CP50978H
- [26] Modelling the metal-on-top effect for Pd clusters on the MgO{100} substrate, I. Atanasov, G. Barcaro, F.R. Negreiros, A. Fortunelli and R.L. Johnston
J. Chem. Phys. (2013) 138, 224703; DOI: 10.1063/1.4807725
- [27] Computational and experimental investigations into the conformations of cyclic tetra-alpha/beta-peptides, M.T. Oakley, E. Oheix, A.F.A. Peacock and R.L. Johnston
J. Chem. Phys. B (2013) 117, 8122-8134; DOI: 10.1021/jp4043039
- [28] Size-dependent subnanometer Pd cluster (Pd₄, Pd₆ and Pd₁₇) water oxidation electrocatalysis, G. Kwon, G.A. Ferguson, C.J. Heard, E.C. Tyo, C. Yin, J. DeBartolo, S. Seifert, R.E. Winans, A.J. Kropf, J. Greeley, R.L. Johnston, L.A. Curtiss, M.J. Pellin and S. Vajda
ACS Nano (2013) 7, 5808-5817; DOI: 10.1021/nn400772s
- [29] An atomistic view of the interfacial structures of AuRh and AuPd nanorods, R.L. Chantry, I. Atanasov, W. Siriwatcharapiboon, B.P. Khanal, E.R. Zubarev, S.L. Horswell, R.L. Johnston and Z.Y. Li
Nanoscale (2013) 5, 7452-7457; DOI: 10.1039/C3NR02560H
- [30] Effect of CO and H adsorption on the compositional structure of binary nanoalloys via DFT modelling, P. S. West, R. L. Johnston, G. Barcaro and A. Fortunelli
Eur. Phys. J D (2013) 67, 165; DOI: 10.1140/epjd/e2013-40257-4
- [31] Direct atomic imaging and density functional theory study of the Au₂₄Pd₁ cluster catalyst, A. Bruma, F.R. Negreiros, S. Xie, T. Tsukuda, R.L. Johnston, A. Fortunelli and Z.Y. Li
Nanoscale (2013) 5, 9620-9625; DOI: 10.1039/c3nr01852k

- [32] Structures of small Ti- and V-doped Pt clusters: a GA-DFT study, P. C. Jennings, and R. L. Johnston
Comp. Theor. Chem. (2013) 1021, 91-100; DOI: 10.1016/j.comptc.2013.06.033
- [33] Evaluation of Photodissociation Spectroscopy as a Structure Elucidation Tool for Isolated Clusters: A Case Study of Ag_4^+ and Au_4^+ , A. Shayeghi, R.L. Johnston and R. Schaefer
Phys. Chem. Chem. Phys. (2013) 15, 19715-19723; DOI: 10.1039/c3cp52160e
- [34] Improving the adsorption of Au atoms and nanoparticles on graphite via Li-intercalation, A.J. Logsdail, R.L. Johnston and J. Akola
J. Phys. Chem. C (2013) 117, 22683-22695; DOI: 10.1021/jp405670v
- [35] Protein structure optimisation with a "Lamarckian" ant colony algorithm, M. T. Oakley, E. G. Richardson, H. Carr and R. L. Johnston
IEEE/ACM Trans. Comp. Bio. Bioinform. (2013) 10, 1548-1552; DOI: 10.1109/TCBB.2013.125
- [36] A DFT study of oxygen dissociation on platinum based nanoparticles, P.C. Jennings, H.A. Aleksandrov, K.M. Neyman and R.L. Johnston
Nanoscale (2014) 6, 1153-1165; DOI: 10.1039/C3NR04750D
- [37] Global Optimization of 8-10 Atom Palladium-Iridium Nanoalloys at the DFT Level, J.B.A. Davis, S.L. Horswell and R.L. Johnston
J. Phys. Chem. A (2014) 118, 208-214; DOI: 10.1021/jp408519z
- [38] Optical and Electronic Properties of Mixed Ag-Au Tetramer Cations, A. Shayeghi, C.J. Heard, R.L. Johnston and R. Schaefer
J. Chem. Phys. (2014) 140, 054312; DOI: 10.1063/1.4863443
- [39] Support and Oxidation Effects on Subnanometer Palladium Nanoparticles, C.J. Heard, S. Vajda, and R. L. Johnston
J. Phys. Chem. C (2014) 118, 3581-3589; DOI: 10.1021/jp411019t
- [40] Energy Landscapes and Global Optimisation of Self-Assembling Cyclic Peptides, M.T. Oakley and R.L. Johnston
J. Chem. Theory Comput. (2014) 10, 1810-1816; DOI: 10.1021/ct500004k
- [41] A Theoretical Study of the Structures and Optical Spectra of Helical Copper-Silver Clusters, C.J. Heard and R.L. Johnston
Phys. Chem. Chem. Phys. (2014) 116, 21039-21048; DOI: 10.1039/c3cp55507k
- *[42] Influence of spin-orbit effects on structures and dielectric properties of neutral lead clusters, D. Götz, A. Shayeghi, R.L. Johnston, P. Schwerdtfeger and R. Schäfer
J. Chem. Phys. (2014) 140, 164313; DOI: 10.1063/1.4872369
- *[43] Structure and solid solution properties of Cu-Ag nanoalloys, I. Atanasov, R. Ferrando and R.L. Johnston,
J. Phys.: Condens. Matter (2014) 26, 275301; DOI: 10.1088/0953-8984/26/27/275301
- *[44] Visualising energy landscapes with metric disconnectivity graphs, L.C. Smeeton, M.T. Oakley and R.L. Johnston,
J. Comput. Chem. (2014) 35, 1481-1490; DOI: 10.1002/jcc.23643
- *[45] $\text{Pd}_n\text{Ag}_{(4-n)}$ and $\text{Pd}_n\text{Pt}_{(4-n)}$ clusters on MgO (100): A density functional surface genetic algorithm investigation, C.J. Heard, S. Heiles, S. Vajda and R.L. Johnston,
Nanoscale (2014) 6, 11777-11788; DOI: 10.1039/c4nr03363a
- *[46] Global minimum search of Ag_{10}^+ with molecular beam optical spectroscopy, A. Shayeghi, R.L. Johnston and R. Schaefer,
J. Chem. Phys. (2014) 141, 181104; DOI: 10.1063/1.4901109
- *[47] DFT studies of oxygen dissociation on the 116-atom platinum truncated octahedron particle, P.C. Jennings, H.A. Aleksandrov, K.M. Neyman and R.L. Johnston,
Phys.Chem.Chem.Phys. (2014) 16, 26539-26545; DOI: 10.1039/C4CP02147A
- *[48] Comparative modelling of chemical ordering in palladium-iridium nanoalloys, J.B.A. Davis, R.L. Johnston, L. Rubinovich and M. Polak,
J. Chem. Phys. (2014) 141, 224307; DOI: 10.1063/1.4903188

From Lev Kantorovich's Group

- [1] Pulling the C60 molecule on a Si(001) surface with an STM tip: A theoretical study, N. Martsinovich and L. Kantorovich,
Phys. Rev. B (2008) 77, 115429; DOI: 10.1103/PhysRevB.77.115429
- [2] H-bonding supramolecular assemblies of PTCDI molecules on the Au(111) surface, M. Mura, F. Silly, G. A. D. Briggs, M. R. Castell and L. Kantorovich,

J. Phys. Chem. C (2009) 113, 21840-21848; DOI: 10.1021/jp908046t

[3] [Experimental and theoretical analysis of H-bonded supramolecular assemblies of PTCDA molecules](#),

M. Mura, X. Sun, F. Silly, H.T. Jonkman, G.A.D. Briggs, M.R. Castell and L.N. Kantorovich, *Phys. Rev. B* (2010) 81, 195412; DOI: 10.1103/PhysRevB.81.195412

[4] [Structure of InSb \(001\) surface](#),

D. Toton, J. He, G. Goryl, J. Kołodziej, S. Godlewski, L. Kantorovich and M. Szymonski, *J. Phys. Cond. Matter* (2010) 22, 265001; DOI: 10.1088/0953-8984/22/26/265001

[5] [Structure of the indium-rich InSb\(001\) surface](#),

G. Goryl, D. Toton, N. Tomaszewska, J.S. Prauzner-Bechcicki, L. Walczak, A. Tejada, A. Taleb-Ibrahimi, L. Kantorovich, E. G. Michel and J.J. Kołodziej, *Phys. Rev. B* (2010) 82, 165311; DOI: 10.1103/PhysRevB.82.165311

[6] [Role of van der Waals interaction in forming molecule-metal junctions: flat organic molecules on the Au\(111\) surface](#),

M. Mura, A. Gulans, T. Thonhauser and L. Kantorovich, *Phys. Chem. Chem. Phys.* (2010) 12, 4759; DOI: 10.1039/b920121a

[7] [Manipulating Si\(100\) at 5 K using qPlus frequency modulated atomic force microscopy: Role of defects and dynamics in the mechanical switching of atoms](#),

A. Sweetman, S. Jarvis, R. Danza, J. Bamidele, L. Kantorovich and P. Moriarty,

Phys. Rev. B (2011) 84, 085426; DOI: 10.1103/PhysRevB.84.085426

[8] [Homochiral Xanthine Quintet Networks Self-Assembled on Au\(111\) Surfaces](#),

M. Yu, J. Wang, M. Mura, Q.-Q. Meng, W. Xu, H. Gersen, E. Lægsgaard, I. Stensgaard, R.E.A. Kelly, J. Kjems, T. R. Linderoth, L. N. Kantorovich, and F. Besenbacher, *ACS Nano* (2011) 8, 6651; DOI: 10.1021/nn202157m

[9] [Chemical tip fingerprinting in scanning probe microscopy of an oxidized Cu\(110\) surface](#),

J. Bamidele, Y. Kinoshita, R. Turanský, S.H. Lee, Y. Naitoh, Y.J. Li, Y. Sugawara, I. Štich, and L. Kantorovich,

Phys. Rev. B (2012) 86, 155422; DOI: 10.1103/PhysRevB.86.155422

[10] [Fabrication of a Complex Two-Dimensional Adenine-Perylene-3,4,9, 10-tetracarboxylic Dianhydride Chiral Nanoarchitecture through Molecular Self-Assembly](#),

X. Sun, M. Mura, H.T. Jonkman, L.N. Kantorovich, and F. Silly,

J. Phys. Chem. C (2012) 116, 2493; DOI: 10.1021/jp2095054

[11] [Complex design of dissipation signals in non-contact atomic force microscopy](#),

J. Bamidele, Y.J. Li, S. Jarvis, Y. Naitoh, Y. Sugawara and L. Kantorovich,

Phys. Chem. Chem. Phys. (2012) 14, 16250-16257; DOI: 10.1039/c2cp43121a

[12] [Critical importance of van der Waals stabilization in strongly chemically bonded surfaces: Cu\(110\):O](#),

J. Bamidele, J. Brndiar, A. Gulans, L. Kantorovich and I. Stich,

J. Chem. Theory and Comput. (2013) 9, 5578-5584; DOI: 10.1021/ct400813d

[13] [Image formation and contrast inversion in NC-AFM imaging of the oxidized Cu\(110\) surfaces](#),

J. Bamidele, Y. Kinoshita, R. Turansky, S.H. Lee, Y. Naitoh, Y.J. Li, Y. Sugawara, I. Stich and L. Kantorovich,

Phys. Rev. B (2014) 90, 035410; DOI: 10.1103/PhysRevB.90.035410

*[14] [Identifying tips for intramolecular NC-AFM imaging via in situ tip fingerprinting](#),

H. Sang, S.P. Jarvis, Z. Zhou, P. Sharp, J. Wang, Y. Wang, and L. Kantorovich,

Scientific Reports (2014) 4, 6678; DOI: 10.1038/srep06678

* [15] [Vertical atomic manipulation with dynamic AFM without tip change via multi-step mechanism](#),

J. Bamidele, S.H. Lee, Y. Kinoshita, R. Turansky, Y. Naitoh, Y.J. Li, Y. Sugawara, I. Stich, and L. Kantorovich,

Nature Comm. (2014) 5, 4476; DOI: 10.1038/ncomms5476

From Moti Lal's Group

[1] [Solvation of metal nanoparticles in a subcritical-supercritical fluid: a computer simulation study](#),

M. Lal, M. Plummer, N.J. Richmond and W. Smith,

J. Phys. Chem. B (2004) 108, 6052-6061; DOI: 10.1021/jp036776e

[2] [Solvent density effects on the solvation behavior and configurational structure of bare and passivated 38-atom gold nanoparticle in supercritical ethane](#),

M. Lal, M. Plummer and W. Smith,

J. Phys. Chem. B (2006) 110, 20879-20888; DOI: 10.1021/jp0633650

[3] [A computer simulation study of the interaction between passivated and bare gold nanoclusters](#),

M. Lal, M. Plummer, J.A. Purton and W. Smith,
Proc. Roy. Soc. A (2011) 467, 1986-2003; DOI: 10.1098/rspa.2010.0513

From Keith McKenna's Group

- [1] [Optical Properties of Nanocrystal Interfaces in Compressed MgO Nanopowders](#),
K. P. McKenna, D. Koller, A. Sternig, N. Siedl, N. Govind, P. Sushko and O. Diwald,
ACS Nano (2011) 5, 3003-3009; DOI: 10.1021/nn200062d
- [2] [Two-dimensional polaronic behavior in the binary oxides \$m\text{-HfO}_2\$ and \$m\text{-ZrO}_2\$](#) ,
K. P. McKenna, M. J. Wolf, A. L. Shluger, S. Lany and A. Zunger,
Phys. Rev. Lett. (2012) 108, 116404; DOI: 10.1103/PhysRevLett.108.116403
- [3] [Exciton formation at solid-solid interfaces: a systematic experimental and ab initio study on compressed MgO nanopowders](#),
A. Sternig, D. Koller, N. Siedl, O. Diwald and K. McKenna,
J. Phys. Chem. C (2012) 116, 10103; DOI: 10.1021/jp3015222
- [4] [Hole trapping at surfaces of \$m\text{-ZrO}_2\$ and \$m\text{-HfO}_2\$ nanocrystals](#),
M. J. Wolf, K. P. McKenna and A. Shluger,
J. Phys. Chem. C (2012) 116, 25888; DOI: 10.1021/jp309525g
- [5] [Crossover from Incoherent to Coherent Electron Tunneling between Defects in MgO](#),
K. P. McKenna and J. Blumberger,
Phys. Rev. B (2012) 86, 245110; DOI: 10.1103/PhysRevB.86.245110
- [6] [Constrained Density Functional Theory Applied to Electron Tunnelling between Defects](#),
J. Blumberger and K. P. McKenna,
Phys. Chem. Chem. Phys. (2013) 15, 2184-2196; DOI: 10.1039/c2cp42537h
- [7] [Structure and electronic properties of polycrystalline dielectrics](#),
K.P. McKenna and A.L. Shluger,
Electrochemical Society Transactions (2013) 54, 243; DOI: 10.1149/05401.0243ecst
- [8] [Grain Boundary Controlled Electron Mobility in Polycrystalline Titanium Dioxide](#),
S. Wallace and K.P. McKenna,
Adv. Mater. Inter. (2014) 1400078, 1-5; DOI: 10.1002/admi.201400078
- *[9] [Polymorphism of dislocation core structures at the atomic scale](#),
Z-C. Wang, M. Saito, K.P. McKenna, and Y. Ikuhara
Nature Communications (2014) 5, 323; DOI: 10.1038/ncomms4239
- *[10] [Optimal stoichiometry for nucleation and growth of conductive filaments in \$\text{HfO}_x\$](#) ,
K.P. McKenna
Modelling and Simulation in Materials Science and Engineering (2014) 22, 025001; DOI: 10.1088/0965-0393/22/2/025001
- *[11] [Electronic and chemical properties of a surface terminated screw dislocation in MgO](#)
K.P. McKenna
Journal of the American Chemical Society (2013) 135, 18859-18865; DOI: 10.1021/ja408342z
- *[12] [Atomic scale structure and properties of highly stable antiphase boundary defects in \$\text{Fe}_3\text{O}_4\$](#) ,
K.P. McKenna, F. Hofer, D. Gilks, V.K. Lazarov, C. Chen, Z. Wang and Y. Ikuhara
Nature Communications (2014) 5, 5740; DOI: 10.1038/ncomms6740

From Angelos Michaelides's Group

- [1] [Ice formation on kaolinite: Lattice match or amphotericism?](#)
X.L. Hu and A. Michaelides,
Surf. Sci. (2007) 601, 3529; DOI: 10.1016/j.susc.2007.09.012
- [2] [Water on the hydroxylated \(001\) surface of kaolinite: From monomer adsorption to a flat 2D wetting layer](#),
X.L. Hu and A. Michaelides,
Surf. Sci. (2008) 602, 960; DOI: 10.1016/j.susc.2007.12.032
- [3] [A one-dimensional ice structure built from pentagons](#),
J. Carrasco, A. Michaelides, M. Forster, S. Haq, R. Raval and A. Hodgson,
Nature Materials (2009) 8, 427-431; DOI: 10.1038/NMAT2403
- [4] [Interfacial water: A first principles molecular dynamics study of a nanoscale water film on salt](#),
L.-M. Liu, M. Krack and A. Michaelides,
J. Chem. Phys. (2009) 130, 234702; DOI: 10.1063/1.3152845
- [5] [Experimental and theoretical study of oxygen adsorption structures on \$\text{Ag}\(111\)\$](#) ,
J. Schnadt, J. Knudsen, X. L. Hu, A. Michaelides, R. T. Vang, K Reuter, Z. Li, E. Lægsgaard, M. Scheffler and F. Besenbacher,

- Phys. Rev. B* (2009) 80, 075424; DOI: 10.1103/PhysRevB.80.075424
- [6] [Chemical accuracy for the van der Waals density functional](#),
J. Klimes, D.R. Bowler and A. Michaelides,
J. Phys.: Condens. Matter (2010) 22, 022201; DOI: 10.1088/0953-8984/22/2/022201
- [7] [Structure and dynamics of liquid water on rutile TiO₂\(110\)](#),
L. Liu, C. Zhang, G. Thornton and A. Michaelides,
Phys. Rev. B - Rapid Communications (2010) 82, 161415(R); DOI: 10.1103/PhysRevB.82.161415
- [8] [Quantum nature of the proton in water-hydroxyl overlayers on metal surfaces](#),
X. Li, M. Probert, A. Alavi and A. Michaelides,
Phys. Rev. Lett. (2010) 104, 066102; DOI: 10.1103/PhysRevLett.104.066102
- [9] [Direct assessment of quantum nuclear effects on hydrogen bond strength by constrained-centroid ab initio path integral molecular dynamics](#),
B. Walker and A. Michaelides,
J. Chem. Phys. (2010) 133, 174306; DOI: 10.1063/1.3505038
- [10] [The kaolinite \(001\) polar basal plane](#),
X. L. Hu and Angelos Michaelides,
Surf. Sci. (2010) 604, 111; DOI: 10.1016/j.susc.2009.10.026
- [11] [A critical assessment of theoretical methods for finding reaction pathways and transition states of surface processes](#),
J. Klimeš, D. R. Bowler and A. Michaelides,
J. Phys.: Condensed Matter (2010) 22, 074203; DOI: 10.1088/0953-8984/22/7/074203
- [12] [Surface energy and surface proton order of the ice Ih basal and prism surfaces](#),
D. Pan, L. M. Liu, G. A. Tribello, B. Slater, A. Michaelides and E. Wang,
J. Phys.: Condensed Matter (2010) 22, 074209; DOI: 10.1088/0953-8984/22/7/074209
- [13] [Proton transfer in adsorbed water dimers](#),
X. L. Hu, J. Klimeš, and A. Michaelides,
Phys. Chem. Chem. Phys. (2010) 12, 3953; DOI: 10.1039/B924422K
- [14] [To wet or not to wet? Dispersion forces tip the balance for water-ice on metals](#),
J. Carrasco, B. Santra, J. Klimes and A. Michaelides,
Phys. Rev. Lett. (2011) 106, 026101; DOI: 10.1103/PhysRevLett.106.026101
- [15] [Quantum nuclear effects on the location of hydrogen above and below the palladium\(100\) surface](#),
C. Zhang and A. Michaelides,
Surface Science (2011) 605, 689–694; DOI: 10.1016/j.susc.2011.01.004
- [16] [Quantum nature of the hydrogen bond](#),
X.Z. Li, B. Walker and A. Michaelides,
Proc. Natl. Acad. Sci. (2011) 108, 6369; DOI: 10.1073/pnas.1016653108
- [17] [Van der Waals density functionals applied to solids](#),
J. Klimeš, D. R. Bowler and A. Michaelides,
Phys. Rev. B (2011) 83, 195131; DOI: 10.1103/PhysRevB.83.195131
- [18] [Melting the ice: on the relation between melting temperature and size for nanoscale ice crystals](#),
Ding Pan, Li-Min Liu, Ben Slater, Angelos Michaelides and Enge Wang,
ACS Nano (2011) 5, 4562; DOI: 10.1021/nn200252w
- [19] [Trends in water monomer adsorption and dissociation on flat insulating surfaces](#),
X. L. Hu, J. Carrasco, J. Klimeš and A. Michaelides,
Phys. Chem. Chem. Phys. (2011) 13, 12447; DOI: 10.1039/C1CP20846B
- [20] [Initial stages of salt dissolution determined with ab initio molecular dynamics](#),
L. M. Liu, A. Laio and A. Michaelides,
Phys. Chem. Chem. Phys. (2011) 13, 12447; DOI: 10.1039/c1cp21077g
- [21] [Hydrogen bonds and van der Waals forces in ice at ambient and high pressures](#),
B. Santra, J. Klimeš, D. Alfè, B. Slater, A. Michaelides, R. Car and M. Scheffler,
Phys. Rev. Lett. (2011) 107, 185701; DOI: 10.1103/PhysRevLett.107.185701
- [22] [Acetone adsorption on ice investigated by X-ray spectroscopy and density functional theory](#),
D. E. Starr, D. Pan, J. T. Newberg, M. Ammann, E. G. Wang, A. Michaelides and H. Bluhm,
Phys. Chem. Chem. Phys. (2011) 13, 19988; DOI: 10.1039/c1cp21493d
- [23] [Visualization of hydrogen bonding and associated chirality in methanol hexamers](#),
T. J. Lawton, J. Carrasco, A. E. Baber, A. Michaelides and E. C. H. Sykes,
Phys. Rev. Lett. (2011) 107, 256101; DOI: 10.1103/PhysRevLett.107.256101
- [24] [Water-hydroxyl phases on an open metal surface: breaking the ice rules](#),

- M. Forster, R. Raval, J. Carrasco, A. Michaelides and A. Hodgson,
Chem. Sci. (2012) 3, 93; DOI: 10.1039/c1sc00355k
- [25] Reply to “Comment on “Structure and Dynamics of liquid water on rutile TiO₂ (110)”,
L.-M. Liu, C. Zhang, G. Thornton and A. Michaelides,
Phys. Rev. B (2012) 85, 167402; DOI: 10.1103/PhysRevB.85.167402
- [26] Non-hexagonal ice at hexagonal surfaces: the role of lattice mismatch,
S. J. Cox, S. M. Kathmann, J. A. Purton, M. J. Gillan, A. Michaelides,
Phys. Chem. Chem. Phys. (2012) 14, 7944; DOI: 10.1039/c2cp23438f
- [27] Nature of proton transport in a water-filled carbon nanotube and in liquid water,
J. Chen, X-Z Li, Q. Zhang, A. Michaelides and E. Wang,
Phys. Chem. Chem. Phys. (2013) 15, 6344; DOI: 10.1039/c3cp50218j
- [28] Classical and quantum ordering of protons in cold solid hydrogen under megabar pressures,
X-Z Li, B. Walker, M. I. J. Probert, C. J. Pickard, R. J. Needs and A. Michaelides,
J. Phys.: Condens. Matter (2013) 25, 085402; DOI: 10.1088/0953-8984/25/8/085402
- [29] The role of van der Waals forces in water adsorption on metals,
J. Carrasco, J. Klimeš and A. Michaelides,
J. Chem. Phys. (2013) 138, 024708; DOI: 10.1063/1.4773901
- [30] Quantum effects in the diffusion of hydrogen on Ru(0001),
E.M. McIntosh, K.T. Wikfeldt, J. Ellis, A. Michaelides and W. Allison,
J. Phys. Chem. Lett. (2013) 4, 1565; DOI: 10.1021/jz400622v
- [31] Insight into the description of van der Waals forces for benzene adsorption on transition metal (111) surfaces,
J. Carrasco, W. Liu, A. Michaelides and A. Tkatchenko,
J. Chem. Phys. (2014) 140, 084704; DOI: 10.1063/1.4866175
- [32] Significant quantum effects in hydrogen activation,
G. Kyriakou, E.R.M. Davidson, G. Peng, L.T. Roling, S. Singh, M.B. Boucher, M.D. Marcinkowski, M. Mavrikakis, A. Michaelides and E.C.H. Sykes,
ACS Nano (2014) 8, 4827; DOI: 10.1021/nn500703k
- *[33] On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures,
B. Santra, J. Klimeš, A. Tkatchenko, D. Alfè, B. Slater, A. Michaelides, R. Car and M. Scheffler
J. Chem. Phys. (2013) 139, 154702; DOI: 10.1063/1.4824481
- *[34] Understanding the role of ions and water molecules in the NaCl dissolution process,
J. Klimeš, D.R. Bowler and A. Michaelides
J. Chem. Phys. (2013) 139, 041103; DOI: 10.1063/1.4840675
- *[35] The microscopic features of heterogeneous ice nucleation may affect the macroscopic morphology of atmospheric ice crystals,
S. J. Cox, Z. Raza, S.M. Kathmann, B. Slater and A. Michaelides
Faraday Discuss. (2013) 167, 389; DOI: 10.1039/C3FD00059A
- *[36] Solvent-induced proton hopping at a water-oxide interface,
G. Tocci and A. Michaelides
J. Phys. Chem. Lett. (2014) 5, 474; DOI: 10.1021/jz402646c
- *[37] Quantum simulation of low-temperature metallic liquid hydrogen,
J. Chen, X.Z. Li, Q. Zhang, M.I.J. Probert, C.J. Pickard, R.J. Needs, A. Michaelides, E. Wang
Nature Comm. (2013) 4, 2064; DOI: 10.1038/ncomms3064
- *[38] Structure and energetics of hydrogen-bonded networks of methanol on close packed transition metal surfaces,
C.J. Murphy, J. Carrasco, T.J. Lawton, M.L. Liriano, A.E. Baber, E.A. Lewis, A. Michaelides and E.C. H. Sykes
J. Chem. Phys. (2014) 141, 014701; DOI: 10.1063/1.4882863

From Barbara Montanari's Group

- [1] Dynamics of Single Fe Atoms in Graphene Vacancies,
A.W. Robertson, B. Montanari, K. He, J. Kim, C.S. Allen, Y.A. Wu, J. Olivier, J. Neethling, N. Harrison, A.I. Kirkland and J.H. Warner,
Nano Lett. (2013) 13, 1468–1475; DOI: 10.1021/nl304495v
- [2] Structural reconstruction of the graphene monovacancy,
A.W. Robertson, B. Montanari, K. He, C. Allen, Y. Wu, N.M. Harrison, A.I. Kirkland, J. Warner,
ACS Nano (2013) 7, 4495-4502; DOI: 10.1021/nn401113r

*[3] Study of the interaction of water with the aqua-soluble dimeric complex [RuCp(PTA)₂-μ-CN-1κC:2κ2N-RuCp(PTA)₂](CF₃SO₃) (PTA = 1,3,5-triaza-7-phosphaadamantane) by neutron and X-ray diffraction in solution,

M. Serrano-Ruiz, S. Imberti, L. Bernasconi, N. Jadagayeva, F. Scalambra and A. Romerosa, *Chem.Comm.* (2014) 50, 11587-11590; DOI: 10.1039/C4CC05225K

From Arash Mostofi's Group

[1] System-size convergence of point defect properties: The case of the silicon vacancy,

F. Corsetti and A.A. Mostofi

Phys. Rev. B (2011) 84, 035209; DOI: 10.1103/PhysRevB.84.035209

[2] A first-principles study of As doping at a disordered Si-SiO₂ interface,

F. Corsetti and A.A. Mostofi

J. Phys.: Condens. Matter (2014) 26, 5, 055002, 1-9; DOI: 10.1088/0953-8984/26/5/055002

[3] Negative-U properties for substitutional Au in Si,

F. Corsetti and A.A. Mostofi

Europhysics Letters (2014) 105, 57006 DOI: 10.1209/0295-5075/105/57006

*[4] Accelerated simulations of aromatic polymers,

R.J. Broadbent, J.S. Spencer, A.A. Mostofi and A.P. Sutton

Molecular Simulation (2014) 112, 2672; DOI: 10.1080/00268976.2014.905719

From Sanghamitra Mukhopadhyay's Group

[1] Influence of background carriers on magnetic properties of Mn-doped dilute magnetic Si,

S. Mukhopadhyay and N.M. Harrison,

J. Mag. Mag. Mat. (2012) 324, 3748; DOI: 10.1016/j.jmmm.2012.06.010

[2] Electronic structures and phonon free energies of LaCoO₃ using hybrid exchange density functional theory,

S. Mukhopadhyay, M.W. Finnis and N.M. Harrison,

Phys. Rev. B. (2013), 87, 125132; DOI: 10.1103/PhysRevB.87.125132

[3] Hydrogen bonding in the organic ferroelectric croconic acid: insights from experiment and first-principles modelling,

F. Fernandez-Alonso, M.J. Gutmann, S. Mukhopadhyay, D.B. Jochym, K. Refson, M. Jura, M. Krzystyniak, M. Jimenez-Ruiz and A. Wagner,

J. Phys. Soc. Japan (2013), 82, SA001; DOI: 10.1143/JPSJS.82SA.SA001

[4] Ferroelectric behaviour in solid croconic acid using neutron scattering and first-principles density functional theory,

S. Mukhopadhyay, M.J. Gutmann, M. Jura, D.B. Jochym, M. Jimenez-Ruiz, S. Sturniolo, K. Refson and F. Fernandez-Alonso,

Chem. Phys. (2013), 427, 95; DOI: 10.1016/j.chemphys.2013.10.008

From Pooja Panchmatia's Group

[1] Manipulation of spin state of iron porphyrin by chemisorption on magnetic substrates,

S. Bhandary, B. Brena, P.M. Panchmatia, I. Brumboiu, M. Bernien, C. Weis, B. Krumme, C. Etz, W. Kuch, H. Wende, O. Eriksson and B. Sanyal,

Phys. Rev. B (2013) 88, 024401; DOI: 10.1103/PhysRevB.88.024401

[2] Synthesis, conductivity and structural aspects of Nd₃Zr₂Li_{7-3x}Al_xO₁₂,

M.A. Howard, O. Clemens, K.S. Knight, P.A. Anderson, S. Hafiz, P.M. Panchmatia and P.R. Slater,

J. Mater. Chem. A (2013) 1, 14013–14022; DOI: 10.1039/c3ta13252h

From Steve Parker's Group

[1] Atomistic modelling of adsorption and segregation at inorganic solid interfaces,

J.P. Allen, W. Greń, M. Molinari, C. Arrouvel, F. Maglia, and S.C. Parker,

Mol. Simul. (2009) 35, 584-608; DOI: 10.1080/08927020902774570

[2] Mechanical properties of ceria nanorods and nanochains; the effect of dislocations, grain-boundaries and oriented attachment,

T.X.T. Sayle, B.J. Inkson, A. Karakoti, A. Kumar, M. Molinari, G. Mobus, S.C. Parker, S. Seal and D.C. Sayle,

Nanoscale (2011) 3, 1823–1837; DOI: 10.1039/C0NR00980F

[3] Sorptive characteristics of organomontmorillonite toward organic compounds: A combined LFERs and molecular dynamics simulation study,

R. Zhu, W. Chen, T.V. Shapley, M. Molinari, F. Ge, and S.C. Parker,

Environ. Sci. Technol. (2011) 45, 6504–6510; DOI: 10.1021/es200211r

[4] [The structure and dynamics of hydrated and hydroxylated magnesium oxide nanoparticles](#),

D. Spagnoli, J.P. Allen and S.C. Parker,

Langmuir (2011) 27, 1821-1829; DOI: 10.1021/la104190d

[5] [Mechanical properties of ceria nanorods and nanochains; the effect of dislocations, grain-boundaries and oriented attachment](#),

T.X.T. Sayle, B.J. Inkson, A. Karakoti, A. Kumar, M. Molinari, G. Möbus, S.C. Parker, S. Seal and D.C. Sayle,

Nanoscale (2011) 3, 1823-1837, DOI: 10.1039/C0NR00980F

[6] [Water adsorption and its effect on the stability of low index stoichiometric and reduced surfaces of ceria](#),

M. Molinari, S.C. Parker, D.C. Sayle and M.S. Islam,

J. Phys. Chem. C (2012) 116 (12), 7073-7082; DOI: 10.1021/jp300576b

[7] [Strain and architecture-tuned reactivity in ceria nanostructures; enhanced catalytic oxidation of CO to CO₂](#),

T.X.T. Sayle, M. Cantoni, U.M. Bhatta, S.C. Parker, S.R. Hall, G. Möbus, M. Molinari, D. Reid, S. Seal and D.C. Sayle,

Chem. Mater. (2012) 24 (10), 1811-1821; DOI: 10.1021/cm3003436

[8] [Environment-mediated structure, surface redox activity and reactivity of ceria nanoparticles](#),

T.X.T. Sayle, M. Molinari, S. Das, U. M. Bhatta, G. Möbus, S.C. Parker, S. Seal and D.C. Sayle,

Nanoscale (2013) 5, 6063-6073, DOI: 10.1039/C3NR00917C

[9] [Modeling the interaction of nanoparticles with mineral surfaces: adsorbed C₆₀ on pyrophyllite](#),

R. Zhu, M. Molinari, T.V. Shapley and S.C. Parker,

J. Phys. Chem. A (2013) 117 (30), 6602-6611, DOI: 10.1021/jp402835v

[10] [Morphology and surface analysis of pure and doped cuboidal ceria nanoparticles](#),

U. Bhatta, D. Reid, T. Sakthivel, T.X.T. Sayle, D.C. Sayle, M. Molinari, S.C. Parker, I.M. Ross, S. Seal and G. Moebus,

J. Phys. Chem. C (2013), 117 (46), 24561–24569, DOI: 10.1021/jp405993v

[11] [Atomistic modelling of the sorption free energy of persistent organic pollutants at clay-water interfaces](#),

T.V. Shapley, M. Molinari, R. Zhu and S.C. Parker,

J. Phys. Chem. C (2013), 117 (47), 24975–24984, DOI: 10.1021/jp410173t

[12] [Structural, electronic and thermoelectric behaviour of CaMnO₃ and CaMnO_{\(3-δ\)}](#),

M. Molinari, D.A. Tompsett, S.C. Parker, F. Azough and R. Freer

J. Mater. Chem. A (2014), 2, 14109-14117, DOI: 10.1039/C4TA01514B

*[13] [Ab initio investigation of the UO₃ polymorphs: structural properties and thermodynamic stability](#),

N.A. Brincat, S.C. Parker, M. Molinari, G.C. Allen and M.T. Storr,

Inorg. Chem. (2014), 53 (23), 12253-12264; DOI: 10.1021/ic500791m

*[14] [Towards modelling clay mineral nanoparticles: the edge surfaces of pyrophyllite and their interaction with water](#),

D.M.S. Martins, M. Molinari, M.A. Gonçalves, J.P. Mirão and S.C. Parker,

J. Phys. Chem. C (2014), 118 (47), 27308–27317, DOI: 10.1021/jp5070853

From Mats Persson's Group

[1] [The interaction of an external charged system with a metal surface: a simplified density functional theory approach](#),

I. Scivetti and M. Persson,

Journal of Physics: Condensed Matter (2013) 25, 355006; DOI: 10.1088/0953-8984/25/35/355006

[2] [Atypical charge redistribution over a charge-transfer monolayer on a metal](#),

T. R. Umbach, I. Fernandez-Torrente, M. Ruby, F. Schulz, C. Lotze, R. Rurali, M. Persson, J.I. Pascual, K.J. Franke,

New Journal of Physics (2013) 15, 083048; DOI: 10.1088/1367-2630/15/8/083048

[3] [Thermally and vibrationally induced tautomerization of single porphycene molecules on a Cu\(110\) surface](#),

T. Kumagai, F. Hanke, S. Gawinkowski, J. Sharp, K. Kotsis, J. Waluk, M. Persson and L. Grill,

Phys. Rev. Lett. (2013) 111, 246101; DOI: 10.1103/PhysRevLett.111.246101

[4] [Controlling intramolecular hydrogen transfer in a porphycene molecule with single atoms or molecules located nearby](#),

T. Kumagai, F. Hanke, S. Gawinkowski, J. Sharp, K. Kotsis, J. Waluk, M. Persson and L. Grill,

Nature Chem. (2013) 6, 41-46; DOI: 10.1038/NCHEM.1804

[5] A simplified density functional theory method for investigating charged adsorbates on an ultrathin, insulating film supported by a metal substrate,

I. Scivetti and M. Persson,

J. Phys.: Condens. Matter (2014) 26, 135003, 1-13; DOI: 10.1088/0953-8984/26/13/135003

*[6] Versatile bottom-up construction of diverse macromolecules on a surface observed by scanning tunnelling microscopy,

S. Haq, F. Hanke, J. Sharp, M. Persson, D.B. Amabilino and R. Raval

ACS Nano (2014) 8, 8856; DOI: 10.1021/nn502388u

From Macro Sacchi's Group

From David Scanlon's Group

*[1] Chemical and structural indicators for large redox potentials in Fe-based positive electrode materials,

B.C. Melot, D.O. Scanlon, M. Reynaud, G. Rousse, J.-N. Chotard, M. Henry and J.M. Tarascon
ACS Applied Materials & Interfaces (2014) 6, 10832; DOI: 10.1021/am405579h

*[2] Understanding the stability of MnPO_4 ,

H. Huang, J. Fang, F. Omenya, M. O'Shea, N.A. Chernova, R. Zhang, Q. Wang, N.F. Quackenbush, L.F.J. Piper, D.O. Scanlon and M.S. Whittingham

J. Mater. Chem. A (2014) 2, 12827; DOI: 10.1039/C4TA00434E

*[3] Low temperature preparation and electrochemical properties of $\text{LiFeSi}_2\text{O}_6$,

S. Zhou, G. King, D.O. Scanlon, M.T. Sougrati and B.C. Melot

J. Electrochem. Soc. (2014) 2, 248; DOI: 10.1149/2.0611410jes

*[4] Solution processing route to multifunctional titania thin films: highly conductive and photocatalytically active Nb:TiO_2 ,

D.S. Bhachu, S. Sathasivam, G. Sankar, D.O. Scanlon, G. Cibir, C.J. Carmalt, I.P. Parkin, G.W. Watson, S.M. Bawaked, A.Y. Obaid, S. Al-Thabaiti and S.N. Basahel

Adv. Funct. Mater. (2014) 24, 5075; DOI: 10.1002/adfm.201400338

*[5] Understanding the defect chemistry of alkali metal strontium silicate solid solutions: insights from experiment and theory,

R.D. Bayliss, S.N. Cook, D.O. Scanlon, S. Fearn, J. Cabana, C. Greaves, J.A. Kilner and S.J. Skinner
J. Mater. Chem. A (2014) 2, 17919; DOI: 10.1039/c4ta04299a

*[6] Valence-band density of states and surface electron accumulation in epitaxial SnO_2 films,

S.K. Vasheghani Farahani, T.D. Veal, J.J. Mudd, D.O. Scanlon, G.W. Watson, O. Bierwagen, M.E. White, J.S. Speck and C.F. McConville

Phys. Rev. B (2014) 90, 155413; DOI: 10.1103/PhysRevB.90.155413

*[7] Interface stoichiometry control to improve device voltage and modify band alignment in $\text{ZnO}/\text{Cu}_2\text{O}$ heterojunction solar cells,

S.S. Wilson, J.P. Bosco, Y. Tolstova, D.O. Scanlon, G.W. Watson, and H.A. Atwater,
Energy Environ. Sci. (2014) 7, 3606; DOI: 10.1039/C4EE01956C

From Alex Shluger's Group

[1] First principles calculations of defects near a grain boundary in MgO ,

K.P. McKenna and A.L. Shluger,

Phys. Rev. B (2009) 79, 224116; DOI: 10.1103/PhysRevB.79.224116

[2] Electronic properties of defects in polycrystalline dielectric materials,

K.P. McKenna and A.L. Shluger,

Microelectronics Engineering (2009) 86, 1751-1755; DOI: 10.1016/j.mee.2009.03.125

[3] Modelling of electron and hole trapping in oxides,

K.P. McKenna, P.V. Sushko, A.V. Kimmel, D. Munoz Ramo and A.L. Shluger,

Modelling Simul. Mater. Sci. Eng. (2009) 17, 084004; DOI: 10.1088/0965-0393/17/8/084004

[4] The interaction of oxygen vacancies with grain boundaries in monoclinic HfO_2 ,

K.P. McKenna and A.L. Shluger,

Applied Physics Letters (2009) 95, 222111; DOI: 10.1063/1.3271184

[5] Interplay between adsorbate diffusion and electron tunneling at an insulating surface,

K.P. McKenna, T. Trevethan and A.L. Shluger,

Phys. Rev. B (2010) 82, 085427; DOI: 10.1103/PhysRevB.82.085427

[6] Electron and hole trapping in polycrystalline metal oxide materials,

K.P. McKenna and A.L. Shluger,

Proceedings of the Royal Society A (2010), DOI: 10.1098/rspa.2010.0518

- [7] Unambiguous determination of the adsorption geometry of a metal-organic complex on a bulk insulator,
K. Lammle, T. Trevethan, A. Schwarz, M. Watkins, A. Shluger and R. Wiesendanger,
Nano Lett. (2010) 10, 2965; DOI: 10.1021/nl101290t
- [8] Grain boundary mediated leakage current in polycrystalline HfO₂ films,
K.P. McKenna, A. Shluger, V. Iglesias, M. Porti, M. Nafria, M. Lanza and G. Bersuker,
Microelectronics Engineering (2011), DOI: 10.1016/j.mee.2011.03.024
- [9] Optical properties of nanocrystal interfaces in compressed MgO nanopowders,
K.P. McKenna, D. Koller, A. Sternig, N. Siedl, N. Govind, P. Sushko and O. Diwald,
ACS Nano (2011), DOI: 10.1021/nn200062d
- [10] Role of water in atomic resolution AFM in solutions
M. Watkins, M.L. Berkowitz, A.L. Shluger, *Phys. Chem. Chem. Phys.* (2011) 13, 12584; DOI: 10.1039/c1cp21021a
- [11] Chemical resolution at ionic crystal surfaces using dynamic atomic force microscopy with metallic tips,
G. Teobaldi, K. Lammle, T. Trevethan, M. Watkins, A. Schwarz, R. Wiesendanger and A.L. Shluger,
Phys. Rev. Lett. (2011) 106, 216102; DOI: 10.1103/PhysRevLett.106.216102
- [12] Models of triplet self-trapped excitons in SiO₂, HfO₂, and HfSiO₄,
D. Munoz Ramo, P.V. Sushko and A.L. Shluger,
Phys. Rev. B (2012) 85, 024120; DOI: 10.1103/PhysRevB.85.024120
- [13] Determining adsorption geometry, bonding, and translational pathways of a metal-organic complex on an oxide surface: co-salen on NiO(001),
A. Schwarz, D.Z. Gao, K. Lammle, J. Grenz, M. Watkins, A.L. Shluger and R. Wiesendanger,
J. Phys. Chem. C (2013) 117, 1105-1112; DOI: 10.1021/jp311702j
- [14] Effects of oxide roughness at metal oxide interface: MgO on Ag(001),
S.L. Ling, M.B. Watkins and A.L. Shluger,
J. Phys. Chem. C (2013) 117, 5075-5083; DOI: 10.1021/jp311141k
- [15] Mechanisms of photodesorption of Br atoms from CsBr surfaces,
M.T.E. Halliday, A.G. Joly, W.P. Hess, P.V. Sushko and A.L. Shluger,
J. Phys. Chem. C (2013) 117, 13502-13509; DOI: 10.1021/jp4036343
- [16] The behaviour of oxygen at metal electrodes in HfO₂ based resistive switching devices,
S.R. Bradley, K.P. McKenna and A.L. Shluger,
Microelectronic Engineering (2013) 109, 346-350; DOI: 10.1016/j.mee.2013.03.132
- [17] A computational study of Si-H bonds as precursors for neutral E' centres in amorphous silica and at the Si/SiO₂ interface
S.L. Ling, A. El-Sayed, F. Lopez Gejo, M.B. Watkins, V.V. Afanas'ev and A. L. Shluger
Microelectronic Engineering (2013) 109, 310-313; DOI: 10.1016/j.mee.2013.03.028
- [18] Identification of intrinsic electron trapping sites in bulk amorphous silica from ab initio calculations,
A. El-Sayed, M.B. Watkins, A.L. Shluger and V.V. Afanas'ev,
Microelectronic Engineering (2013) 109, 68-71; DOI: 10.1016/j.mee.2013.03.027
- [19] Structural dynamics of laser-irradiated gold nanofilms,
S.L. Daraszewicz, Y. Giret, N. Naruse, Y. Murooka, J. Yang, D.M. Duffy, A.L. Shluger and K. Tanimura,
Phys. Rev. B (2013) 88, 184101; DOI: 10.1103/PhysRevB.88.184101
- [20] Determination of transient atomic structure of laser-excited materials from time-resolved diffraction data,
Y. Giret, N. Naruse, S.L. Daraszewicz, Y. Murooka, J. Yang, D.M. Duffy, A.L. Shluger and K. Tanimura,
Applied Phys. Lett. (2013) 103, 25, 253107; DOI: 10.1063/1.4847695
- [21] Using metallic noncontact atomic force microscope tips for imaging insulators and polar molecules: tip characterization and imaging mechanisms,
D.Z. Gao, J. Grenz, Josef, M.B. Watkins, F.F. Canova, A. Schwarz, R. Wiesendanger and A.L. Shluger,
ACS Nano (2014) 8, 5339; DOI: 10.1021/nn501785q
- [22] Nature of intrinsic and extrinsic electron trapping in SiO₂,
A.-M. El-Sayed, M.B. Watkins, V.V. Afanas'ev and A.L. Shluger,
Phys. Rev. B (2014) 89, 125201; DOI: 10.1103/PhysRevB.89.125201
- *[23] Nonthermal solid-to-solid phase transitions in tungsten,
Y. Giret, S.L. Daraszewicz, D.M. Duffy, A.L. Shluger and K. Tanimura

Phys. Rev. B (2014) 90, 094103; DOI: 10.1103/PhysRevB.90.094103

*[24] [Determination of the electron-phonon coupling constant in tungsten](#),
S.L. Daraszewicz, Y. Giret, H. Tanimura, D.M. Duffy, A.L. Shluger and K. Tanimura
Appl. Phys. Lett. (2014) 105, 023112; DOI: 10.1063/1.4890413

* [25] [Molecular design and control over the morphology of self-assembled films on ionic substrates](#),
A. Amrous, F. Bocquet, L. Nony, F. Para, C. Loppacher, S. Lamare, F. Palmino, F. Cherioux, D.Z. Gao, F.F. Canova, M.B. Watkins and A.L. Shluger,
Adv. Mater. Int. (2014) 1, 15606-15613; DOI: 10.1002/admi.201400414

From Ben Slater's Group

[1] [A theoretical examination of known and hypothetical clathrate hydrate materials](#),
G.A. Tribello and B. Slater,

J. Chem. Phys. (2009) 131, 024703; DOI: 10.1063/1.3142503

[2] [Zeolitic imidazole frameworks: structural and energetics trends compared with their zeolite analogues](#),

D.W. Lewis, A.R. Ruiz-Salvador, A.Gómez, L.M. Rodriguez-Albelo, F.X. Coudert, B. Slater, A.K. Cheetham and C. Mellot-Draznieks,
Cryst. Eng. Comm. (2009) 11, 2272–2276; DOI: 10.1039/b912997a

[3] [On thin ice: surface order and disorder during pre-melting](#),
C.L. Bishop, D. Pan, L.M. Liu, G.A. Tribello, A. Michaelides, E.G. Wang and B. Slater,
Faraday Discuss. (2009) 141, 277–292; DOI: 10.1039/b807377p

[4] [Point defects at the ice \(0001\) surface](#),

M. Watkins, J. VandeVondele and B. Slater,
Proc. Nat. Acad. Sci. (2010) 107, 12429–12434; DOI: 10.1073/pnas.1001087107

[5] [Flexibility in a metal-organic framework material controlled by weak dispersion forces: The bistability of MIL-53\(Al\)](#),

A.M. Walker, B. Civalleri, B. Slater, C. Mellot-Draznieks, F. Cora, C.M. Zicovich-Wilson, G. Roman-Perez, J.M. Soler and J.D. Gale,
Angew. Chem. Int. Ed. (2010) 49, 7501–7503; DOI: 10.1002/anie.201002413

[6] [Unstitching the nanoscopic mystery of zeolite crystal formation](#),

R. Brent, P. Cubillas, S.M. Stevens, K.E. Jelfs, A. Umemura, J.T. Gebbie, B. Slater, O. Terasaki, M.A. Holden and M.W. Anderson,
J. Am. Chem. Soc. (2010) 132, 13858–13868; DOI: 10.1021/ja105593v

[7] [Proton ordering in cubic ice and hexagonal ice; a potential new ice phase-XIc](#),

Z. Raza, D. Alfè, C. G. Salzmann, J. Klimeš, A. Michaelides and B. Slater,
Phys. Chem. Chem. Phys. (2011) 13, 19788; DOI: 10.1039/C1CP22506E

[8] [Conformer interconversion in a switchable porous organic cage](#),

K.E. Jelfs, F. Schiffmann, J.T.A. Jones, B. Slater, F. Cora and A.I. Cooper,
Phys. Chem. Chem. Phys. (2011) 13 (45), 20081-20085; DOI: 10.1039/c1cp22527h

[9] [Large variation of vacancy formation energies in the surface of crystalline ice](#),

M. Watkins, D. Pan, E. G. Wang, A. Michaelides, J. VandeVondele and B. Slater,
Nature Mater. (2011) 10, 794-798; DOI: 10.1038/NMAT3096

[10] [Modular and predictable assembly of porous organic molecular crystals](#),

Cooper, A. I. et al.,
Abs. Am. Chem. Soc. (2012) 242; DOI: ????

[11] [Comparison of the relative stability of zinc and lithium-boron zeolitic imidazolate frameworks](#),

R. Galvelis, B. Slater, A.K. Cheetham and C. Mellot-Draznieks,
Cryst. Eng. Comm. (2012) 14 374–378; DOI: 10.1039/c1ce05854a

[12] [A polar corundum oxide displaying weak ferromagnetism at room temperature](#),

M.-R. Li, U. Adem, S.R.C. McMitchell, Z. Xu, C.I. Thomas, J.E. Warren, D.V. Giap, H. Niu, X. Wan, R.G. Palgrave, F. Schiffmann, F. Cora, B. Slater, T.L. Burnett, M.G. Cain, A.M. Abakumov, G. van Tendeloo, M.F. Thomas, M.J. Rosseinsky and J.B. Claridge,
J. Am. Chem. Soc. (2012) 134, 3737–3747; DOI: 10.1021/ja208395z

From Alexey Sokol's Group

[1] [On the problem of cluster structure diversity and the value of data mining](#),

A.A. Sokol, C.R.A. Catlow, M. Miskufova, S.A. Shevlin, A.A. Al-Sunaidi, A. Walsh and S.M. Woodley,
Phys. Chem. Chem. Phys. (2010) 12, 8438-8445; DOI: 10.1039/c0cp00068j

[2] [Advances in computational studies of energy materials](#),

C.R.A. Catlow, Z.X. Guo, M. Miskufova, S.A. Shevlin, A.G.H. Smith, A.A. Sokol, A. Walsh, D.J. Wilson and S.M. Woodley,

Phil. Trans. Roy. Soc. A (2010) 368, 3379-3456; DOI: 10.1098/rsta.2010.0111

[3] [Microscopic origins of electron and hole stability in ZnO](#),

C.R.A. Catlow, A.A. Sokol and A. Walsh,

Chemical Communications (2011); DOI: 10.1039/c1cc10314h

[4] [Characterisation of hydrogen dissociation over aluminium-doped zinc oxide using an efficient massively parallel framework for QM/MM calculations](#),

T. W. Keal, P. Sherwood, G. Dutta, A. A. Sokol and C. R. A. Catlow,

Proceedings of the Royal Society A (2011); DOI: 10.1098/RSPA.2010.0613

[5] [Prediction on the existence and chemical stability of cuprous fluoride](#),

A. Walsh, C.R.A. Catlow, R. Galvelis, D.O. Scanlon, F. Schiffmann, A.A. Sokol and S.M. Woodley,

Chem. Sci. (2012) 3, 2565–2569; DOI: 10.1039/c2sc20321a

[6] [Embedded-cluster calculations in a numeric atomic orbital density-functional theory framework](#),

D. Berger, A. J. Logsdail, H. Oberhofer, M.R. Farrow, C.R.A. Catlow, P. Sherwood, A.A. Sokol, V. Blum, K. Reuter,

J. Chem. Phys. (2014) 141, 024105, 1–11; DOI: 10.1063/1.4885816

*[7] [Bulk ionisation potentials and band alignments from 3D periodic calculations as demonstrated on rocksalt oxides](#),

A.J. Logsdail, D.O. Scanlon, C.R.A. Catlow and A.A. Sokol

Phys. Rev. B. (2014) 90, 155106-1-8; DOI: 10.1103/PhysRevB.90.155106

Peter Sushko's Group

[1] [Thermodynamic instability at the stoichiometric LaAlO₃/SrTiO₃\(001\) interface](#),

L. Qiao, T.C. Droubay, V. Shutthanandan, Z. Zhu, P.V. Sushko and S.A. Chambers,

J. Physics: Condens. Matter (2010) 22, 312201; DOI: 10.1088/0953-8984/22/31/312201

[2] [Models of stoichiometric and oxygen-deficient surfaces of subnanoporous 12CaO · 7Al₂O₃](#), P.V.

Sushko, A.L. Shluger, Y. Toda, M. Hirano and H. Hosono,

P. Roy. Soc. A – Math. Phy. (2011) 467, 2066–2083; DOI: 10.1098/rspa.2010.0560

[3] [Band alignment, built-in potential and the absence of conductivity at the LaCrO₃/SrTiO₃\(001\) heterojunction](#),

S.A. Chambers, L. Qiao, T.C. Droubay, T.C. Kaspar, B.W. Arey and P.V. Sushko,

Phys. Rev. Lett. (2011) 107, 206802; DOI: 10.1103/PhysRevLett.107.206802

[4] [Selective response of mesoporous silicon to adsorbants with nitro groups](#),

J.A. McLeod, E.Z. Kurmaev, P.V. Sushko, T.D. Boyko, I.A. Levitsky and A. Moewes,

Chem. – Eur. J. (2012) 18, 2912–2922; DOI: 10.1002/chem.201102084

[5] [Spectroscopic characterization of a multiband complex oxide: insulating and conducting cement 12CaO · 7Al₂O₃](#),

J.A. McLeod, A. Buling, E.Z. Kurmaev, P.V. Sushko, M. Neumann, L.D. Finkelstein, S.-W. Kim, H. Hosono and A. Moewes,

Phys. Rev. B (2012) 85, 045204; DOI: 10.1103/PhysRevB.85.045204

[6] [Tuning optical properties of complex oxides: examples of 12CaO · 7Al₂O₃ mayenite and LaCrO₃ perovskite](#),

P.V. Sushko,

Proceedings of SPIE (2012) 8263, 826310; Oxide-based Materials and Devices III, Editors: F.H. Teherani; D.C. Look, D.J. Rogers; ISBN: 9780819489067; DOI: 10.1117/12.912844

[7] [High performance LiNi_{0.5}Mn_{1.5}O₄ spinel controlled by Mn³⁺ concentration and site disorder](#),

J. Xiao, X. Chen, P.V. Sushko, M.L. Sushko, L. Kovarik, J. Feng, Z. Deng, J. Zheng, G.L. Graff, Z. Nie, D. Choi, J. Liu, J.-G. Zhang and M.S. Whittingham,

Adv. Mater. (2012) 24, 2109–2116; DOI: 10.1002/adma.201104767

[8] [Defect-mediated lattice relaxation and domain stability in ferroelectric oxides](#),

A.V. Kimmel, P.M. Weaver, M.G. Cain and P.V. Sushko,

Phys. Rev. Lett. (2012) 117601, 109; DOI: 10.1103/PhysRevLett.109.117601

[9] [Neutral and charged oxygen vacancies induce two-dimensional electron gas near SiO₂/BaTiO₃ interfaces](#),

A.V. Kimmel, J. Iniguez, M.G. Cain and P.V. Sushko,
J. Phys. Chem. Lett. (2013) 4, 333; DOI: 10.1021/jz301948k
[10] [Multiband optical absorption controlled by lattice strain in thin-film LaCrO₃](#),
P.V. Sushko, L. Qiao, M. Bowden, T. Varga, G.J. Exarhos, F.K. Urban III, D. Barton and S.A. Chambers,
Phys. Rev. Lett. (2013) 110, 077401; DOI: 10.1103/PhysRevLett.110.077401
[11] [Activation and splitting of carbon dioxide on the surface of an inorganic electride material](#),
Y. Toda, H. Hirayama, N. Kuganathan, A. Torrisi, P.V. Sushko and H. Hosono,
Nature Communications (2013) 4, 2378; DOI: 10.1038/ncomms3378
[12] [Oxygen vacancies and ordering of d-levels control voltage suppression in oxide cathodes: the case of spinel LiNi_{0.5}Mn_{1.5}O_{4-δ}](#),
P.V. Sushko, K.M. Rosso, J.-G. Zhang, J. Liu and M.L. Sushko,
Adv. Func. Mater. (2013) 23, 44, 5530-5535; DOI: 10.1002/adfm.201301205
[13] [Enhanced N₂ dissociation on Ru-loaded inorganic electride](#),
N. Kuganathan, H. Hosono, A.L. Shluger and P.V. Sushko,
J. Am. Chem. Soc. (2014) 136, 2216-2219; DOI: 10.1021/ja410925g

From Antonio Tilocca's Group

[1] [Structure and dynamics of bioactive phosphosilicate glasses and melts from ab initio molecular dynamics simulations](#),
A. Tilocca,
Phys. Rev B (2007) 76, 224202; DOI: 10.1103/PhysRevB.76.224202
[2] [Exploring the Surface of Bioactive Glasses: Water Adsorption and Reactivity](#),
A. Tilocca and A.N. Cormack,
J. Phys. Chem. C (2008) 112, 11936; DOI: 10.1021/jp803541j
[3] [Short- and medium-range structure of multicomponent bioactive glasses and melts: An assessment of the performances of shell-model and rigid-ion potentials](#),
A. Tilocca,
J. Chem. Phys. (2008) 129, 084504; DOI: 10.1063/1.2972146
[4] [Modeling the water-bioglass interface by ab-initio molecular dynamics simulations](#),
A. Tilocca and A.N. Cormack,
ACS Applied Materials & Interfaces (2009) 1, 1324; DOI: 10.1021/am900198t
[5] [Sodium migration pathways in multicomponent silicate glasses: Car-Parrinello Molecular Dynamics simulations](#),
A. Tilocca,
J. Chem. Phys. (2010) 133, 014701; DOI: 10.1063/1.3456712
[6] [Surface signatures of bioactivity: MD simulations of 45S and 65S silicate glasses](#),
A. Tilocca and A.N. Cormack,
Langmuir 26, 545 (2010); DOI: 10.1021/la902548f
[7] [Short-range structure of yttrium aluminosilicate glass for cancer radiotherapy: Car-Parrinello molecular dynamics calculations](#),
J.K. Christie and A. Tilocca,
Advanced Engineering Materials (2010) 12, B326; DOI: 10.1002/adem.200980081
[8] [The initial stages of bioglass dissolution: a Car-Parrinello molecular dynamics study of the glass-water interface](#),
A. Tilocca and A.N. Cormack,
Proc. R. Soc. A (2011) 467, 2102; DOI: 10.1098/rspa.2010.0519
[9] [The fluorine environment in bioactive glasses: ab initio molecular dynamics simulations](#)
J.K. Christie, A. Pedone, M.C. Menziani and A. Tilocca,
Journal of Physical Chemistry B (2011) 115, 2038; DOI: 10.1021/jp110788h
[10] [Bioactive glasses as potential radioisotope vectors for in-situ cancer therapy: investigating the structural effects of yttrium](#)
J. Christie, J. Malik and A. Tilocca,
Phys. Chem. Chem. Phys. (2011) 13, 17749; DOI: 10.1039/C1CP21764J
[11] [Molecular dynamics simulations of a bioactive glass nanoparticle](#),
A. Tilocca,
J. Mater. Chem. (2011) 21, 12660; DOI: 10.1039/C1JM11927C

[12] Integrating biological activity into radioisotope vectors: molecular dynamics models of yttrium-doped bioactive glasses,

J. K. Christie and A. Tilocca,

J. Mater. Chem. (2012) 22, 12023; DOI: 10.1039/C2JM31561K

[13] DFT-GGA and DFT+U simulations of thin water layers on reduced TiO₂ anatase,

A. Tilocca and A. Selloni,

J. Phys. Chem. C (2012) 116, 9114; DOI: 10.1021/jp301624v

[14] Molecular dynamics simulations and structural descriptors of radioisotope glass vectors for in situ radiotherapy,

J. K. Christie and A. Tilocca,

J. Phys. Chem. B (2012) 116, 12614; DOI: 10.1021/jp304200f

[15] Cooling rate and size effects on the medium-range structure of multicomponent oxide glasses simulated by molecular dynamics,

A. Tilocca,

J. Chem. Phys. (2013) 139, 114501; DOI: 10.1063/1.4821150

From Kostya Trachenko's Group

[1] Modelling high-energy radiation damage in nuclear and fusion applications,

K. Trachenko, E. Zarkadoula, I.T. Todorov, M.T. Dove, D.J. Dunstan and K. Nordlund,
Nucl. Instr. Methods Phys. Res. B (2012) 277, 6–13; DOI: 10.1016/j.nimb.2011.12.058

[2] The nature of high-energy radiation damage in iron,

E. Zarkadoula, S.L. Daraszewicz, D.M. Duffy, M.A. Seaton, I.T. Todorov, K. Nordlund, M.T. Dove and K. Trachenko,

J. Phys.: Condens. Matter (2013) 25, 125402; DOI: 10.1088/0953-8984/25/12/125402

From Aron Walsh's Group

[1] Defect processes in a PbS metal organic framework: A quantum-confined hybrid semiconductor,
A. Walsh,

J. Phys. Chem. Lett. (2010) 1, 1284–1287; DOI: 10.1021/jz100312y

[2] Surface oxygen vacancy origin of electron accumulation in indium oxide,

A. Walsh,

Appl. Phys. Lett. (2011) 98, 261910; DOI: 10.1063/1.3604811

[3] Effects of reduced dimensionality on the electronic structure and defect chemistry of semiconducting hybrid organic-inorganic PbS solids,

A. Walsh,

Proc. Roy. Soc. A (2011) 467, 1970-1985; DOI: 10.1098/rspa.2010.0514

[4] Structural diversity and electronic properties of Cu₂SnX₃ (X = S, Se): A first-principles investigation,
Y.T. Zhai, S.Y. Chen, J.H. Yang, H.J. Xiang, X.G. Gong, A. Walsh, J. Kang and S.H. Wei,

Phys. Rev. B (2011) 84, 075213; DOI: 10.1103/PhysRevB.84.075213

[5] Thickness dependence of the strain, band gap and transport properties of epitaxial In₂O₃ thin films grown on Y-stabilised ZrO₂(111),

K.H.L. Zhang, V.K. Lazarov, T.D. Veal, F.E. Oropeza, C.F. McConville, R.G. Egdell and A. Walsh,

J. Phys.-Condensed Matt. (2011) 23, 334211; DOI: 10.1088/0953-8984/23/33/334211

[6] Multi-component transparent conducting oxides: progress in materials modelling,

A. Walsh, J.L.F. Da Silva and S.-H. Wei,

J. Phys.-Condensed Matt. (2011) 23, 334210; DOI: 10.1088/0953-8984/23/33/334210

[7] Nature of the band gap and origin of the conductivity of PbO₂ revealed by theory and experiment,

D.O. Scanlon, A.B. Kehoe, G.W. Watson, M.O. Jones, W.I.F. David, D.J. Payne, R.G. Egdell, P.P. Edwards and A. Walsh,

Phys. Rev. Lett. (2011) 107, 246402; DOI: 10.1103/PhysRevLett.107.246402

[8] Surface structure of In₂O₃(111) (1 x 1) determined by density functional theory calculations and low energy electron diffraction,

K. Pussi, A. Matilainen, V.R. Dhanak, A. Walsh, R.G. Egdell and K.H.L. Zhang,

Surf. Sci. (2012) 606, 1-6; DOI: 10.1016/j.susc.2011.07.014

[9] Synthesis, characterization, and calculated electronic structure of the crystalline metal-organic polymers [Hg(SC₆H₄S)(en)]_n and [Pb(SC₆H₄S)(dien)]_n,

D.L. Turner, K.H. Stone, P.W. Stephens, A. Walsh, M.P. Singh and T.P. Vaid,

Inorg. Chem. (2012) 51, 370-376; DOI: 10.1021/ic201779a

[10] Bandgap engineering of ZnSnP₂ for high-efficiency solar cells,

D.O. Scanlon and A. Walsh,
Applied Phys. Lett. (2012) 100, 251911; DOI: 10.1063/1.4730375

[11] Structural and electronic properties of CuSbS_2 and CuBiS_2 : potential absorber materials for thin-film solar cells,
J.T.R. Dufton, A. Walsh, P.M. Panchmatia, L.M. Peter, D. Colombara and M.S. Islam,
Phys. Chem. Chem. Phys. (2012) 14, 7229–7233; DOI: 10.1039/c2cp40916j

[12] A photoactive titanate with a stereochemically active Sn lone pair: Electronic and crystal structure of Sn_2TiO_4 from computational chemistry,
L. Burton and A. Walsh,
J. Sol. State Chem. (2012) 196, 157; DOI: 10.1016/j.jssc.2012.06.013

[13] Conductive metal–organic frameworks and networks: fact or fantasy?
C. Hendon, D. Tiana and A. Walsh,
Phys. Chem. Chem. Phys. (2012) 14, 13120; DOI: 10.1039/C2CP41099K

[14] PbO_2 : from semi-metal to transparent conducting oxide by defect chemistry control
A. Walsh, A.B. Kehoe, D.J. Temple, G.W. Watson and D.O. Scanlon,
Chem. Commun. (2013) 49, 448; DOI: 10.1039/c2cc35928f

[15] Thermodynamic and electronic properties of tuneable II–VI and IV–VI semiconductor based metal–organic frameworks from computational chemistry C
H. Hendon, D. Tiana, T.P. Vaid and A. Walsh,
J. Mater. Chem. C (2013) 1, 95; DOI: 10.1039/c2tc00108j

[16] Polymorphism of indium oxide: materials physics of orthorhombic In_2O_3 ,
A. Walsh and D. O. Scanlon,
Phys. Rev. B (2013) 88, 161201; DOI: 10.1103/PhysRevB.88.161201

[17] Structural and electronic properties of hybrid perovskites for high-efficiency thin-film photovoltaics from first-principles,
F. Brivio, A. B. Walker and A. Walsh,
APL Mater. (2013) 1, 042111; DOI: 10.1063/1.4824147

[18] Dielectric response of Fe_2O_3 crystals and thin films,
R. A. Lunt, A. J. Jackson and A. Walsh,
Chem. Phys. Lett. (2013) 586, 67; DOI: 10.1016/j.cplett.2013.09.023

[19] Helical frontier orbitals of conjugated linear molecules,
C. H. Hendon, D. Tiana, A. Murray, D. A. Carbery and A. Walsh,
Chem. Sci. (2013) 4, 4278; DOI: 10.1039/c3sc52061g

[20] Limits to doping of wide band gap semiconductors,
A. Walsh, J. Buckeridge, C. R. A. Catlow, A. J. Jackson, T. W. Keal, M. Miskufova, P. Sherwood, S. A. Shevlin, M. B. Watkins, S. M. Woodley and A. A. Sokol,
Chem. Mater. (2013) 25, 2924; DOI: 10.1021/cm402237s

[21] Engineering the optical response of the titanium-MIL-125 Metal–Organic Framework through ligand functionalization,
C. H. Hendon, D. Tiana, M. Fontecave, C. Sanchez, L. D'arras, C. Sassoeye, L. Rozes, C. Mellot-Draznieks and A. Walsh,
J. Am. Chem. Soc. (2013) 135, 10942; DOI: 10.1021/ja405350u

[22] Microscopic origin of the optical processes in blue sapphire,
J.K. Bristow, S.C. Parker, C.R.A. Catlow, S.M. Woodley and A. Walsh,
Chem. Commun. (2013) 49, 5259; DOI: 10.1039/c3cc41506f

[23] Electron excess in alkaline earth sub-nitrides: 2D electron gas or 3D electride?
A. Walsh and D. O. Scanlon,
J. Mat. Chem. C (2013) 1, 3525; DOI: 10.1039/c3tc30690a

[24] Band alignment in SnS thin-film solar cells: Possible origin of the low conversion efficiency,
L.A. Burton and A. Walsh,
Appl. Phys. Lett. (2013) 102, 132111; DOI: 10.1063/1.4801313

[25] Thermal physics of the lead chalcogenides PbS , PbSe , and PbTe from first principles,
J.M. Skelton, S.C. Parker, A. Togo, I. Tanaka and A. Walsh,
Phys. Rev. B (2014) 89, 205203, 1–10; DOI: 10.1103/PhysRevB.89.205203

[26] Crystal electron binding energy and surface work function control of tin dioxide,
K.T. Butler, J. Buckeridge, C.R.A. Catlow and A. Walsh,
Phys. Rev. B (2014) 89, 115320, 1–6; DOI: 10.1103/PhysRevB.89.115320

[27] Origin of deep subgap states in amorphous indium gallium zinc oxide: Chemically disordered coordination of oxygen,

S. Sallis, K.T. Butler, N.F. Quackenbush, D.S. Williams, M. Junda, D.A. Fischer, J.C. Woicik, N.J. Podraza, B.E. White Jr., A. Walsh and L.F.J. Piper,
Appl. Phys. Lett. (2014) 104, 232108; DOI: 10.1063/1.4883257

[28] Atomistic origins of high-performance in hybrid halide perovskite solar cells,
J.M. Frost, K.T. Butler, F. Brivio, C.H. Hendon, M. van Schilfgaarde and A. Walsh,
Nano Letters (2014) 14, 5, 2584-2590 DOI: 10.1021/nl500390f

[29] Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells,
J.M. Frost, K.T. Butler and A. Walsh,
APL Materials (2014) 2, 8, 081506 DOI: 10.1063/1.4890246

[30] Ab initio thermodynamic model of $\text{Cu}_2\text{ZnSnS}_4$,
A.J. Jackson and A. Walsh,
Journal of Materials Chemistry A (2014) 2, 21, 7829-7836 DOI: 10.1039/C4TA00892H

[31] Relativistic quasiparticle self-consistent electronic structure of hybrid halide perovskite photovoltaic absorbers,
F. Brivio, K.T. Butler, A. Walsh and M. van Schilfgaarde,
Physical Review B (2014) 89, 15, 155204 DOI: 10.1103/PhysRevB.89.155204

[32] Energetics, thermal isomerisation and photochemistry of the linkage-isomer system $[\text{Ni}(\text{Et}_4\text{dien})(\eta^2\text{-O,ON})(\eta^1\text{-NO}_2)]$,
J.M. Skelton, R. Crespo-Otero, L.E. Hatcher, S.C. Parker, P.R. Raithby and A. Walsh,
Cryst. Eng. Comm. (2014) ????? ; DOI: 10.1039/C4CE01411A

[33] Atomistic origin of the enhanced crystallization speed and n-type conductivity in Bi-doped Ge-Sb-Te phase change materials,
J.M. Skelton, A.R. Pallipurath, T.H. Lee and S.R. Elliott,
Advanced Functional Materials (2014) ????? ; DOI: 10.1002/adfm.201401202

[34] Transferable force field for metal-organic frameworks from first-principles,
J.K. Bristow, D. Tiana, A. Walsh,
J. Chem. Theory Comput. (2014) 10, 4644-4652; DOI: 10.1021/ct500515h

[35] Ligand design for long-range magnetic ordering in metal-organic frameworks,
D. Tiana, C.H. Hendon, A. Walsh,
Chem. Commun. (2014) ????? ; DOI: 10.1039/C4CC06433J

[36] The role of dissolved cations in coffee extraction,
C.H. Hendon, L. Colonna-Dashwood and M. Colonna-Dashwood,
J. Agric. Food Chem. (2014) 62, 4947, DOI: 10.1021/JF501687C

[37] Three-electron two-centred bonds and the stabilisation of cationic sulfur radicals,
C.H. Hendon, D.R. Carbey and A. Walsh,
Chemical Science (2014) 5, 1390-1395; DOI: 10.1039/c3sc53432d

[38] Electronic chemical potentials of porous metal-organic frameworks,
K.T. Butler, C.H. Hendon and A. Walsh,
J. Am. Chem. Soc. (2014) 236, 2703; DOI: 10.1021/ja4110073

From Graeme Watson's Group

[1] Computational screening of trivalent dopants in CeO_2 for improved high-k dielectric behaviour,
P.R.L. Keating, D.O. Scanlon and G.W. Watson,
J. Mater. Chem. C (2013) 1, 1093-1098; DOI: 10.1039/C2TC00385F

[2] Understanding the defect chemistry of tin monoxide,
J.P. Allen, D.O. Scanlon, L.F.J. Piper and G.W. Watson,
J. Mater. Chem. C (2013) 1, 8194-8208; DOI: 10.1039/C3TC31863J

[3] Origin of the bipolar doping behaviour of SnO from X-ray spectroscopy and density functional theory,
N.F. Quackenbush, J.P. Allen, D.O. Scanlon, S. Sallis, J.A. Hewlett, A.S. Nandur, B. Chen, K.E. Smith, C. Weiland, D.A. Fischer, J.C. Woicik, B.E. White, G.W. Watson and L.F.J. Piper,
Chem. Mater. (2013) 25, 3114; DOI: 10.1021/cm401343a

[4] Occupation matrix control of d- and f-electron localisations using DFT + U,
J.P. Allen and G.W. Watson,
Phys. Chem. Chem. Phys. (2014) DOI: 10.1039/c4cp01083c

[5] The nature of oxygen states on the surfaces of CeO_2 and La-doped CeO_2 ,
P.R.L. Keating, D.O. Scanlon and G.W. Watson,
Chem. Phys. Lett. (2014) 608, 239-243; DOI: 10.1016/j.cplett.2014.05.094

From David Willock's Group

- [1] Enantioselective binding of structural epoxide isomers by a chiral vanadyl Salen complex; A pulsed EPR, cw-ENDOR and DFT investigation,
D.M. Murphy, I.A. Fallis, E. Carter, D.J. Willock, J. Landon, S. Van Doorslaer and E. Vinck,
Phys. Chem. Chem. Phys. (2009) 11, 6757-6769; DOI: 10.1039/b907807j
- [2] CO bond cleavage on supported nano-gold during low temperature oxidation,
A.F. Carley, D.J. Morgan, N. Song, M. W. Roberts, S.H. Taylor, J.K. Bartley, D.J. Willock, K.L. Howard and G.J. Hutchings,
Phys. Chem. Chem. Phys. (2011) 13, 2528-2538; DOI: 10.1039/c0cp01852j
- [3] The decomposition of H₂O₂ over the components of Au/TiO₂ catalysts,
A. Thetford, G.J. Hutchings, S.H. Taylor and D.J. Willock,
Proc. Roy. Soc. A, Mat. Phys and Eng., (2011) 467, 1885-1899; DOI: 10.1098/rspa.2010.0561
- [4] A periodic DFT study of the activation of O₂ by Au nanoparticles on α -Fe₂O₃,
K.L. Howard and D.J. Willock,
Faraday Disc. (2011) 152 (1), 135-151; DOI: 10.1039/c1fd00026h
- [5] Enantioselective hydrogenation of α -ketoesters: An in situ surface-enhanced Raman spectroscopy (SERS) study,
R.J. Taylor, Y.X. Jiang, N.V. Rees, G.A. Attard, E.L. Jeffery, and D.J. Willock,
J. Phys. Chem. C (2011) 115, 21363-21372; DOI: 10.1021/jp208403g
- [6] Direct catalytic conversion of methane to methanol in aqueous medium by using copper-promoted Fe-ZSM-5,
C. Hammond, M.M. Forde, M. Hasbi Ab Rahim, A. Thetford, Q. He, R.L. Jenkins, N. Dimitratos, J.A. Lopez-Sanchez, N.F. Dummer, D.M. Murphy, A.F. Carley, S.H. Taylor, D.J. Willock, E.E. Stangland, J. Kang, H. Hagen, C.J. Kiely and G.J. Hutchings,
Angew. Chem. (2012) 51, 5129-5133; DOI: 10.1002/anie.201108706
- *[7] The adsorption and dissociation of CO on Fe(111),
S. Booyens, M. Bowker and D.J. Willock
Surf. Sci. (2014), 625, 69-83; DOI: 10.1016/j.susc.2014.02.019
- *[8] Impact of co-adsorbed oxygen on crotonaldehyde adsorption over gold nanoclusters: A computational study,
C. D. Zeinalipour-Yazdi, D. J. Willock, A. Machado, K. Wilson and A. F. Lee
Phys. Chem. Chem. Phys. (2014), 16, 11202–11210. DOI: 10.1039/C3CP53691B
- *[9] Spectroscopic and atomic force studies of the functionalisation of carbon surfaces: new insights into the role of the surface topography and specific chemical states.
C. Buono, P.R.Davies, R.J. Davies, T. Jones, J. Kulhavy, R. Lewis, D.J. Morgan, N. Robinson and D.J. Willock,
Faraday Discussions (2014) 173, 257-272; DOI: 10.1039/c4fd00061g

From Scott Woodley's Group

- [1] Construction of nano- and microporous frameworks from octahedral bubble clusters,
S.M. Woodley, M.B. Watkins, A.A. Sokol, S.A. Shevlin and C.R.A. Catlow
Phys. Chem. Chem. Phys. (2009) 11, 3176-3185; DOI: 10.1039/b902600b
- [2] Bubbles and microporous frameworks of silicon carbide,
M.B. Watkins, S.A. Shevlin, A.A. Sokol, B. Slater, C.R.A. Catlow and S.M. Woodley
Phys. Chem. Chem. Phys. (2009) 11, 3186-3200; DOI: 10.1039/b902603g
- [3] Structure Prediction of Ternary Oxide Sub-Nanoparticles,
S.M. Woodley
Mater. Manu. Proc. (2009) 24, 255-264; DOI: 10.1080/10426910802675848
- [4] Modelling nano-clusters and nucleation,
C.R.A. Catlow, S.T. Bromley, S. Hamad, M. Mora-Fonz, A.A. Sokol and S.M. Woodley
Phys. Chem. Chem. Phys. (2010) 12, 786-811; DOI: 10.1039/b916069h
- [5] Evolutionary structure prediction and electronic properties of indium oxide nanoclusters,
A. Walsh and S.M. Woodley
Phys. Chem. Chem. Phys. (2010) 12, 8446-8453; DOI: 10.1039/c0cp00056f
- [6] Exploration of multiple energy landscapes for zirconia nanoclusters,
S.M. Woodley, S Hamad and C.R.A. Catlow
Phys. Chem. Chem. Phys. (2010) 12, 8454-8465; DOI: 10.1039/c0cp00057d
- [7] Electronic and Optical Properties of Doped and Undoped (TiO₂)_n Nanoparticles,
S.A. Shevlin and S.M. Woodley,
J. Phys. Chem. C (2010) 114, 17333-17343; DOI: 10.1021/jp104372j
- [8] Atomistic and electronic structure of (X₂O₃)_n nanoclusters; n=1-5, X = B, Al, Ga, In and Tl,

S.M. Woodley

Proc. Roy. Soc. A (2011) 467, 2020-2042; DOI: 10.1098/rspa.2011.0009

[9] [Magnetic properties of Fe₂GeMo₃N; an experimental and computational study](#),

P.D. Battle, L.A. Sviridov, R.J. Woolley, F. Grandjean, G.J. Long, C.R.A. Catlow, A.A. Sokol, A. Walsh and S.M. Woodley

J. Mater. Chem. (2012) 22, 15606-15613; DOI: 10.1039/c2jm32574h

[10] [Introducing k-point parallelism into VASP](#),

A. Maniopoulou, E.R.M. Davidson, R. Grau-Crespo, A. Walsh, I.J. Bush, C.R.A. Catlow and S.M. Woodley

Comp. Phys. Commun. (2012) 183, 1696-1701; DOI: 10.1016/j.cpc.2012.03.009

[11] [Equation of state of CaMnO₃; a combined experimental and computational study](#),

W. Paszkowicz, S.M. Woodley, P. Piszora, B. Bojanowski, J. Pietosa, Y. Cerenius, S. Carlson and C. Martin

Appl. Phys. A (2013) 112, 839–845; DOI: 10.1007/s00339-013-7577-7

[12] [From stable ZnO and GaN clusters to novel double bubbles and frameworks](#),

M.R. Farrow, J. Buckeridge, C.R.A. Catlow, A.J. Logsdail, D.O. Scanlon, A.A. Sokol and S.M. Woodley

Inorganics (2014) 2, 248-263; DOI: 10.3390/inorganics2020248

*[13] [Double bubbles: a new structural motif for enhanced electron–hole separation in solids](#),

M.R. Farrow, J. Buckeridge, C.R.A. Catlow, A.J. Logsdail, D.O. Scanlon, A.A. Sokol and S.M. Woodley

Phys. Chem. Chem. Phys. (2014) 16, 21098-21105; DOI: 10.1039/c4cp01900h

*[14] [Structure prediction of nanoclusters; a direct or a pre-screened search on the DFT energy landscape?](#)

M.R. Farrow, Y. Chow and S.M. Woodley

Phys. Chem. Chem. Phys. (2014) 16, 21119-21134; DOI: 10.1039/c4cp01825g

From Martijn Zwijnenburg's Group

[1] [Optical excitations in stoichiometric uncapped ZnS nanostructures](#),

M.A. Zwijnenburg

Nanoscale (2011) 3, 3780-3787; DOI: 10.1039/c1nr10486a

[2] [Photoluminescence in semiconductor nanoparticles: an atomistic view of excited state relaxation in nanosized ZnS](#),

M.A. Zwijnenburg

Nanoscale (2012) 4, 3711-3717; DOI: 10.1039/c2nr30191a

[3] [Elucidating the microscopic origin of the unique optical properties of polypyrene](#),

M.A. Zwijnenburg

J. Phys. Chem. C (2012) 116, 20191-20198; DOI: 10.1021/jp305146p

[4] [Long range coupling between defect centres in inorganic nanostructures: Valence alternation pairs in nanoscale silica](#),

M.A. Zwijnenburg, F. Illas and S.T. Bromley

J. Chem. Phys. (2012) 137, 154313; DOI: 10.1063/1.4758461

[5] [Excited state localisation cascades in inorganic semiconductor nanoparticles](#),

M.A. Zwijnenburg

Phys. Chem. Chem. Phys. (2013) 15, 11119; DOI: 10.1039/c3cp50800e

[6] [Coupled cluster calculations on TiO₂ nanoclusters](#),

E. Berardo, H.-S. Hu, K. Kowalski, and M.A. Zwijnenburg

J. Chem. Phys. (2013) 139, 064313; DOI: 10.1063/1.4817536

[7] [Shedding light on structure–property relationships for conjugated microporous polymers: the importance of rings and strain](#),

M.A. Zwijnenburg, G. Cheng, T.O. McDonald, K.E. Jelfs, J.X. Jiang, S. Ren, T. Hasell, F. Blanc, A.I. Cooper and D.J. Adams

Macromolecules (2013) 46, 7696; DOI: 10.1021/ma401311s

[8] [Shining a light on s-triazine-based polymers](#),

C. Butchosa, T.O. McDonald, A.I. Cooper, D.J. Adams and M.A. Zwijnenburg,

J. Phys. Chem. C (2014) 118, 4314-4324; DOI: 10.1021/jp411854f

[9] [Modeling excited states in TiO₂ nanoparticles: on the accuracy of a TD-DFT based description](#),

E. Berardo, H.-S. Hu, S.A. Shevlin, S.M. Woodley, K. Kowalski and M.A. Zwijnenburg

J. Chem. Theory Comput., (2014) 10, 1189-1199; DOI: 10.1021/ct4010273

[10] [Polymeric watersplitting photocatalysts; a computational perspective on the water oxidation](#)

conundrum,

P. Guiglion, C. Butchosa and M.A. Zwijnenburg

J. Mater. Chem. (2014) 2, 11996; DOI: 10.1039/C4TA02044H

*[11] [Optical excitation of MgO nanoparticles; A computational perspective,](#)

M.C.C. Wobbe, A.K. Kerridge and M.A. Zwijnenburg

Phys. Chem. Chem. Phys. (2014), 16, 22052-22061, DOI: 10.1039/C4CP03442B

*[12] [Carbon nitride photocatalysts for water splitting: a computational perspective,](#)

C. Butchosa, P. Guiglion, M.A. Zwijnenburg,

J. Phys. Chem. C (2014) 118, 24833–24842; DOI: 10.1021/jp507372n

*[13] [Modeling excited states in TiO₂ nanoparticles: on the accuracy of a TD-DFT based description,](#)

E. Berardo, H.S. Hu, S.A. Shevlin, S.M. Woodley, K. Kowalski, M.A. Zwijnenburg,

J. Chem. Theo. Comput. (2014) 10, 1189–1199; DOI: 10.1021/ct4010273