PROCEEDINGS OF THE ROYAL SOCIETY A MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

High-performance computing in the chemistry and physics of materials

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Proc. R. Soc. A published online 20 April 2011
doi: 10.1098/rspa.2011.0191

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FirstCite® e-publishing

Proc. R. Soc. A
doi:10.1098/rspa.2011.0191
Published online

INTRODUCTION

High-performance computing in the chemistry and physics of materials

High performance computing (HPC) is now a key enabling technology in almost all areas of contemporary science and engineering. Indeed, HPC now allows the development of increasingly detailed, reliable and predictive models of complex systems and problems. The field of materials chemistry and physics has been a particularly fruitful area of application of HPC-enabled modelling. The articles in this issue highlight some of the most significant current areas in this rapidly expanding field and also aim to show how recent improvements in both hardware and software are enabling new scientific applications.

Progress in materials chemistry and physics requires knowledge of structure, electronic properties and reactivity often of multi-component systems. These challenges are evident in the articles addressing the themes of *surface and interfacial science and reactivity*. Key issues in catalytic science are addressed in the articles of Thetford *et al.* (2011) on hydrogen peroxide decomposition and Keal *et al.* (2011) on hydrogen dissociation on oxides. Both studies illustrate the mechanistic detail which may now be obtained by the application of methods based on density functional theory (DFT) as illustrated in figure 1. Grau-Crespo *et al.* (2011) address the important issue of surface segregation in ceria/zirconia solid solutions—a problem of importance in the applications of these materials in auto-exhaust catalysis. While different areas of interfacial science are addressed by Martinez *et al.* (2011) who model interfacial surfactant monolayers; and by Irrera & de Leeuw (2011) who employ DFT-based techniques to probe the complex structures formed by the adsorption of uracil on gold surfaces.

Several papers report detailed investigations of complex *nano-particulate systems*. Walsh (2011) explores the effects of dimensionality on the widely studied hybrid organic–inorganic materials; while both Lal *et al.* (2011) and Tran & Johnston (2011) model metal nano-clusters, with the former addressing the differences between bare gold clusters and those which have been passivated by sorbed thiols (figure 2); and the latter the structures and properties of gold–platinum alloy clusters. The growing field of oxide nano-cluster science is addressed by Woodley (2011) who reports an extensive series of predictions of the structures and electronic properties of sesquioxide nano-clusters.

The properties of *defective solids* remain a core area of materials chemistry and physics. Several papers illustrate the information that can now be obtained on both structural and electronic properties of defects using modelling techniques.

One contribution to a Special feature 'High-performance computing in the chemistry and physics of materials'.

Received 25 March 2011
Accepted 25 March 2011

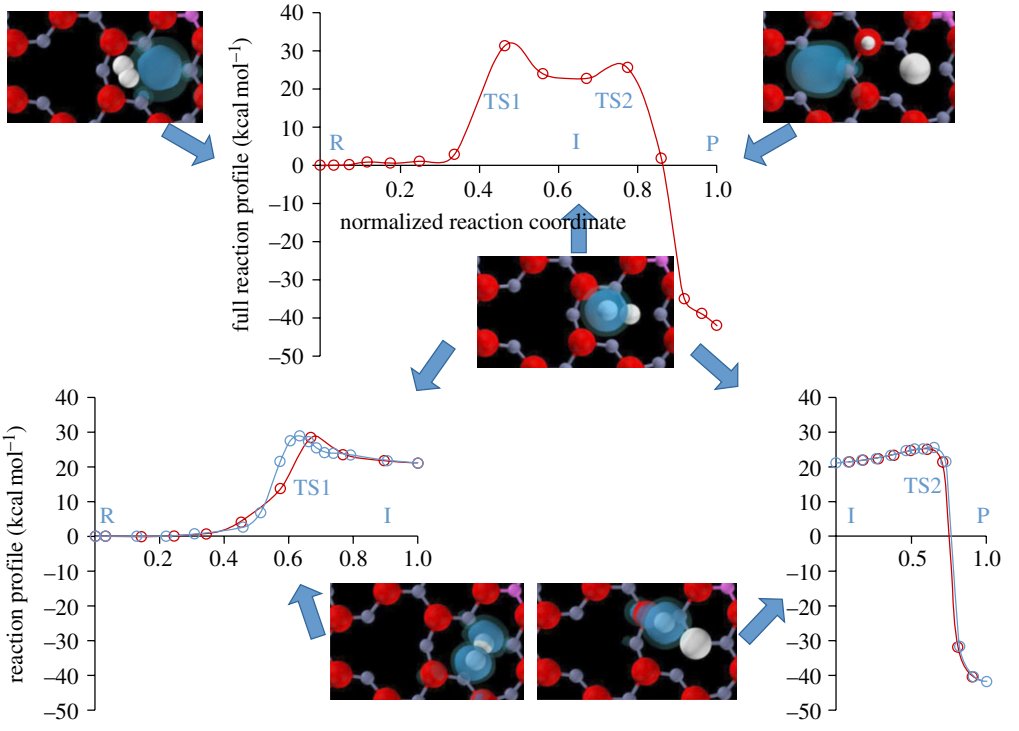

Figure 1. Energy profiles for hydrogen dissociation over zinc oxide (R, reactant; P, product; I, intermediate; TS1 and TS2, first and second transition states). Red, initial run; blue, zoom in. Taken from Keal *et al.* (2011). (Online version in colour.)

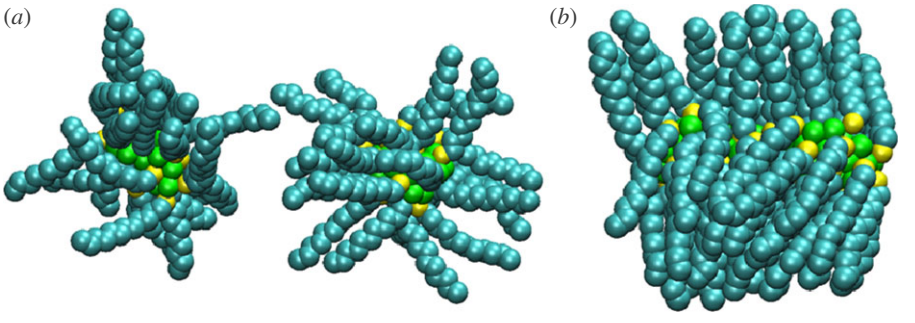

Figure 2. Merger of passivated nano-clusters in ethane solvent at 347 K, with inter-particle distances (*a*) 38 Å and in vacuum at 290 K, with inter-particle distances (*b*) 14 Å. Colour scheme: yellow, gold atoms; green, sulphur atoms; turquoise, CH_2 or CH_3 (united atoms). Taken from Lal *et al.* (2011). (Online version in colour.)

McKenna & Shluger (2011) model the electronic properties of grain boundaries and dislocations in polycrystalline materials (figure 3)—problems of importance in micro-electronics and photocatalysis; and Mulroue & Duffy (2011) examine the effects of charge localization on defect formation and migration energies in oxides—a topic that has often been discussed but regarding which there has

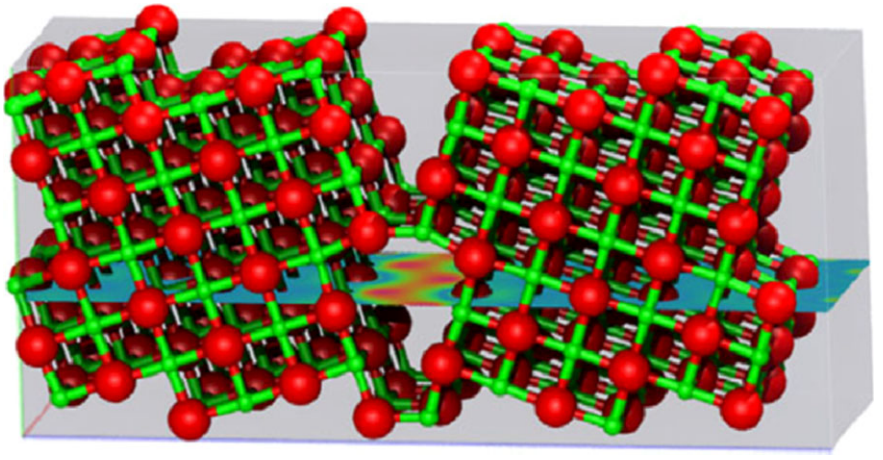

Figure 3. The supercell used to model the (310)[001] tilt grain boundary in MgO, which contains a plot of electron density, within a plane perpendicular to the interface, that shows an electron confined inside the dislocation pipe (red represents high electron density). Taken from McKenna & Shluger (2011). (Online version in colour.)

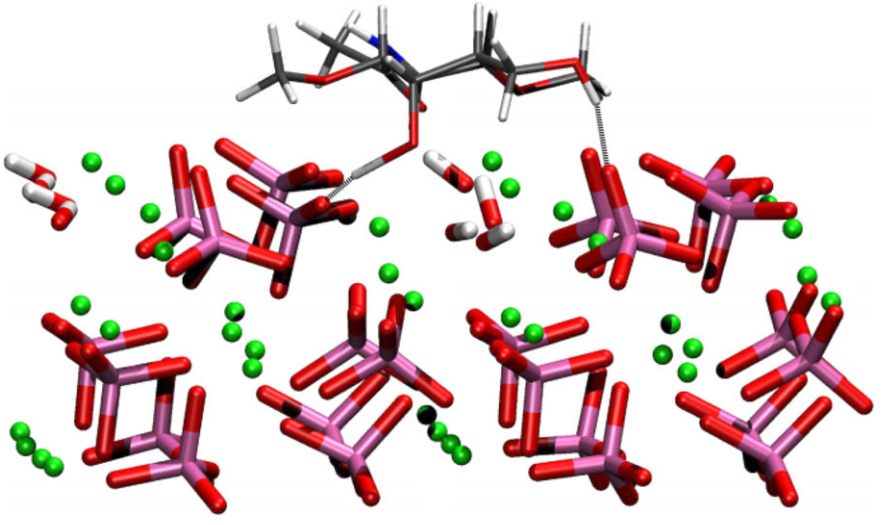

Figure 4. Adsorptions of methylated *N*-acetylgalactosamine on the (0110) surface of hydroxyapatite. Hydrogen bonds from hydroxy groups to phosphate groups are indicated by broken lines. Ca, green; O, red; P, purple; H, white; C, grey; N, blue. Taken from Streeter & de Leeuw (2011). (Online version in colour.)

previously been little quantitative information. The interplay between surface and defect properties is the theme of the paper from Sushko *et al.* (2011), which investigates the optoelectronic CaO/Al_2O_3 material.

Biomaterials science is explored in two articles: Streeter & de Leeuw (2011) model the interactions between saccharides and hydroxyapatite (figure 4)—a factor that may control bone formation; while Tilocca & Cormack (2011) use

ab initio dynamics to model the early stages of bioglass dissolution. The ability of simulation techniques to embrace these complex multi-component systems illustrates well the growing scope of materials modelling using HPC techniques.

Finally, the importance of innovation in software development is clear from the articles of Bush *et al.* (2011) and Keal *et al.* (2011), which describe how the CRYSTAL and ChemShell codes, which perform electronic structure and hybrid calculations on periodic and defective solids, have been optimized for implementation on massively parallel computing platforms.

The science reported in this volume has been critically dependent on the availability of state-of-the-art hardware; and all the work reported has exploited the UK's national high-performance computing facilities—over two and a half thousand processors on the HPC*x* service (December 2002–January 2010) and currently over 40 000 cores on the HECToR service provided by UoE HPC*x* Ltd. at the University of Edinburgh (UoE), Cray Inc. and NAG Ltd., and funded by the Office of Science and Technology through Engineering and Physical Sciences Research Council's (EPSRC) High End Computing Programme. The work has also profited from the investments in software development; and all contributing authors are members of the UK Materials Chemistry HPC Consortium (http://www.ucl.ac.uk/klmc/mcc), which is also funded by EPSRC and which aims to exploit HPC technologies in materials physics and chemistry. We hope that the issue demonstrates the power of HPC-enabled techniques in this field.

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