EDITORIAL

1883

High performance computing in materials chemistry

This issue of *Journal of Materials Chemistry* focuses on recent developments in the use of high performance computing for contemporary modelling studies in materials chemistry. Richard Catlow and Scott M. Woodley, Guest Editors, introduce the issue and highlight the key aspects of the field.

FEATURE ARTICLES

1885

Terascale materials modelling on high performance system HPCx


The HPCx UoE Ltd national computing resource HPCx terascale team works in collaboration with scientists and code developers to optimize and develop materials chemistry codes (for example, GAMESS-UK shown here) to achieve efficient exploitation of large-scale computational resources and thus facilitate new science.
Journal of Materials Chemistry

www.rsc.org/materials

Journal of Materials Chemistry is a weekly, international journal that publishes high impact work covering all aspects of the chemistry of novel materials in all forms, particularly materials associated with new technologies. Coverage of the field is broad and includes the design and synthesis of materials, their characterization, processing, modelling, properties and applications.

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FEATURE ARTICLES

1894

**Planar nucleic acid base super-structures**

R. E. A. Kelly* and L. N. Kantorovich

We review a method relying on assembling super-structures made of DNA bases and stabilised by hydrogen bonding using the knowledge of how the individual molecules form dimers.

PAPERS

1906

*Ab initio* studies of aluminium fluoride surfaces

A. Wander, C. L. Bailey, S. Mukhopadhyay, B. G. Searle and N. M. Harrison

Aluminium fluorides have great potential as strong Lewis acid catalysts in a number of industrial processes such as Cl/F exchange reactions.

1911

**DL_POLY_3: new dimensions in molecular dynamics simulations via massive parallelism**

Ilian T. Todorov,* William Smith, Kostya Trachenko and Martin T. Dove

Massive parallelism with excellent speed-up and highly optimised memory usage; cutting edge numerical algorithms and methodologies; excellent portability—the ultimate general purpose MD simulation package for large scale simulations.

1919

**QM/MM modelling of the TS-1 catalyst using HPCx**


Mixed quantum/classical modelling studies reveal that active titanium sites in TS-1 adopt a stable tripodal configuration, which can be formed from the hydrolysis and inversion of tetrahedral sites in Ti-silicalite.
Properties of small TiO$_2$, ZrO$_2$ and HfO$_2$ nanoparticles
S. M. Woodley,* S. Hamad, J. A. Mejias and C. R. A. Catlow

Ground state structures, based on DFT, and infrared spectra are predicted and compared for (MO$_2$)$_n$, where $n = 1$ to 8 and M is one of three isovalent cations.

Polydispersity in oligomeric low dosage gas hydrate inhibitors
Robert W. Hawtin and P. Mark Rodger*

This paper presents the first molecular-level study of the influence of tacticity and conformation on the activity of low dosage hydrate inhibitors. PDMAEMA is shown to promote nucleation, with linear conformations generating slower nucleation and growth than helical forms.

The effect of cation coordination on the properties of oxygen vacancies in FeSbO$_4$

We investigate the dependence of the oxygen vacancy properties on the cation coordination of the removed oxygen atom in iron antimonate FeSbO$_4$, an important catalyst for the selective oxidation of hydrocarbons.

Structural and electronic properties of modified sodium and soda-lime silicate glasses by Car–Parrinello molecular dynamics
Antonio Tilocca* and Nora H. de Leeuw

Car–Parrinello molecular dynamics simulations elucidated structural and electronic properties of modified silicate glasses, relevant to the technological applications of these materials; in particular, the local environment of Na and Ca ions has been determined with high accuracy.
Hydrogen bond structure and vibrational spectrum of water at a passivated metal nanoparticle
Kafui Tay and Fernando Bresme*
Molecular Dynamics computer simulations show that gold passivated nanoparticles (~3 nm diameter) in water exhibit weak dewetting, similar to that observed in extended hydrophobic surfaces. The nanoparticle–water interface is characterised by a reduction in the number of hydrogen bonds compared to bulk water and by the existence of OH dangling bonds.

Parallel multi-band k·p code for electronic structure of zinc blend semiconductor quantum dots
Stanko Tomicć,* Andrew G. Sunderland and Ian J. Bush
A parallel implementation of the multi-band k·p code has been developed for the electronic structure and optical properties calculation of conventional and dilute nitrogen zinc blend semiconductor quantum dots.

Li sites and phase stability in TiO₂-anatase and Zr-doped TiO₂-anatase
Marina V. Koudriachova* and N. M. Harrison
Doping anatase TiO₂ with zirconium decreases its intercalation potential.

Calculations on the adsorption of Au to MgO surfaces using SIESTA
Rudy Coquet, Graham J. Hutchings, Stuart H. Taylor and David J. Willock*
Auₙ (n = 1, 2, and 10) on MgO is stabilised at defect sites. The adsorption of these species at point and extended defects is compared.
1989

Hydrogen adsorption and diffusion on Pt \{111\} and PtSn \{111\}
Joanne Fearon and Graeme W. Watson*
Addition of Sn to the Pt \{111\} surface results in substantial differences for the mobility of H on the surface. Nudged elastic band calculations show H follows a path that avoids interaction with the Sn atoms.

1997

Molecular dynamics simulations of the interaction between the surfaces of polar solids and aqueous solutions
Dino Spagnoli, David J. Cooke, Sebastien Kerisit and Stephen C. Parker*
Atomistic simulation techniques allow the speciation of metal ion complexes at mineral/electrolyte interfaces to be explored.

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