

Journal of Materials Chemistry

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ISSN 0959-9428 CODEN JMACEP 16(20) 1873–2012 (2006)



Cover

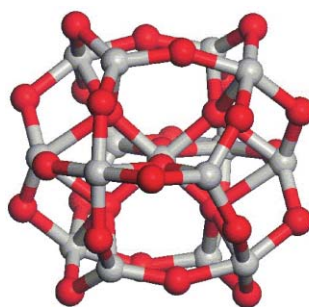
See Kafui Tay and Fernando Bresme, pp. 1956–1962.
Molecular dynamics computer simulation snapshot of the hydrogen bond structure of interfacial water around a passivated gold metal nanoparticle of 3 nm diameter. Image reproduced by permission of Fernando Bresme from *J. Mater. Chem.*, 2006, 16, 1956.

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.



Ground state structure of $(\text{TiO}_2)_{15}$

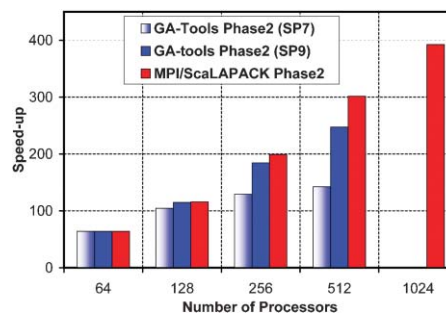
FEATURE ARTICLES

1885

Terascale materials modelling on high performance system HPCx

M. Plummer,* J. Hein, M. F. Guest, K. J. D'Mellow, I. J. Bush, K. Refson, G. J. Pringle, L. Smith and A. Trew

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.



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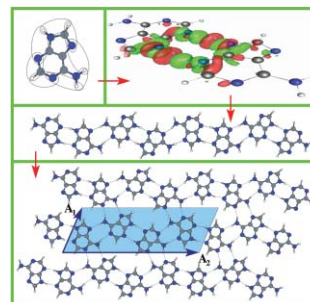
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1894

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.



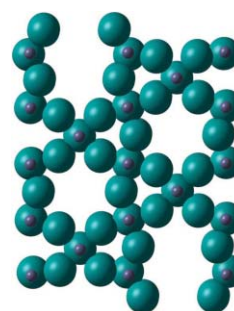
PAPERS

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.

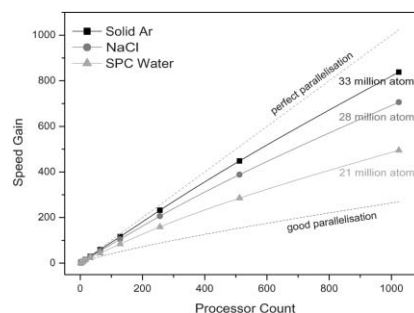


1911

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.

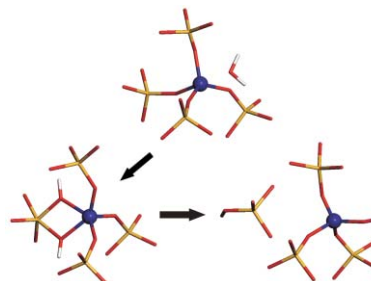


1919

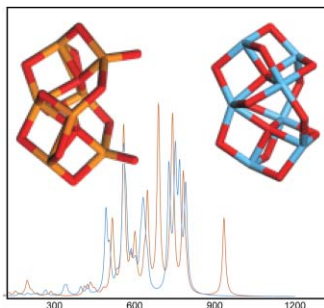
QM/MM modelling of the TS-1 catalyst using HPCx

Judy To, Paul Sherwood, Alexey A. Sokol, Ian J. Bush, C. Richard A. Catlow, Huub J. J. van Dam, Samuel A. French and Martyn F. Guest

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.



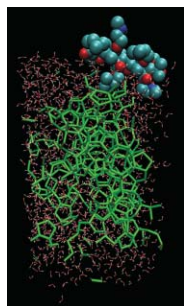
1927

**Properties of small TiO₂, ZrO₂ and HfO₂ nanoparticles**

S. M. Woodley,* S. Hamad, J. A. Mejías and C. R. A. Catlow

Ground state structures, based on DFT, and infrared spectra are predicted and compared for (MO₂)_n, where *n* = 1 to 8 and M is one of three isovalent cations.

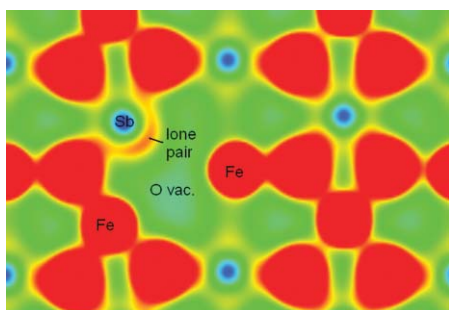
1934

**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.

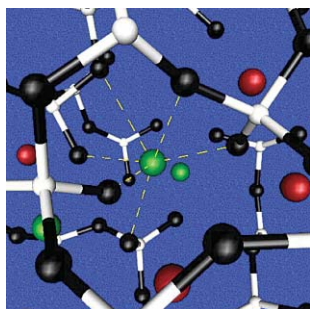
1943

**The effect of cation coordination on the properties of oxygen vacancies in FeSbO₄**

Ricardo Grau-Crespo,* Ibério de P. R. Moreira, Francesc Illas, Nora H. de Leeuw and C. Richard A. Catlow

We investigate the dependence of the oxygen vacancy properties on the cation coordination of the removed oxygen atom in iron antimonate FeSbO₄, an important catalyst for the selective oxidation of hydrocarbons.

1950

**Structural and electronic properties of modified sodium and soda-lime silicate glasses by Car–Parrinello molecular dynamics**

Antonio Tilocca* and Nora H. de Leeuw

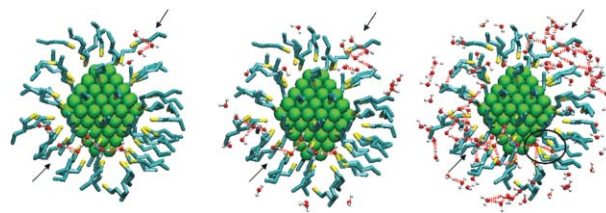
Car–Parrinello molecular dynamics simulations elucidated structural and electronic properties of modified silicate glasses, relevant to the technological applications of these materials; in particular, the local environment of Na and Ca ions has been determined with high accuracy.

1956

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.

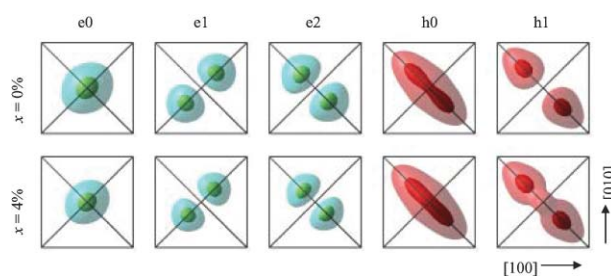


1963

Parallel multi-band $\mathbf{k}\cdot\mathbf{p}$ code for electronic structure of zinc blend semiconductor quantum dots

Stanko Tomić,* Andrew G. Sunderland and Ian J. Bush

A parallel implementation of the multi-band $\mathbf{k}\cdot\mathbf{p}$ code has been developed for the electronic structure and optical properties calculation of conventional and dilute nitrogen zinc blend semiconductor quantum dots.

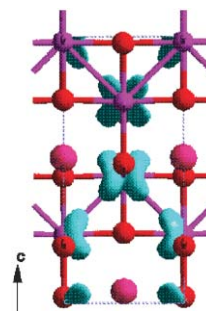


1973

Li sites and phase stability in TiO_2 -anatase and Zr-doped TiO_2 -anatase

Marina V. Koudriachova* and N. M. Harrison

Doping anatase TiO_2 with zirconium decreases its intercalation potential.

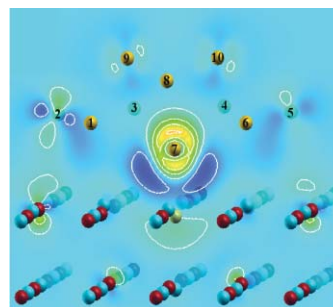


1978

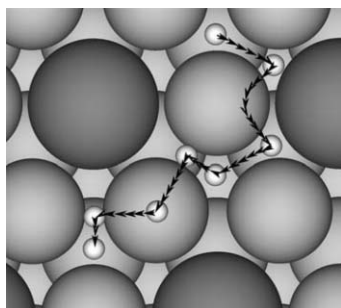
Calculations on the adsorption of Au to MgO surfaces using SIESTA

Rudy Coquet, Graham J. Hutchings, Stuart H. Taylor and David J. Willock*

Au_n ($n = 1, 2$, and 10) on MgO is stabilised at defect sites. The adsorption of these species at point and extended defects is compared.



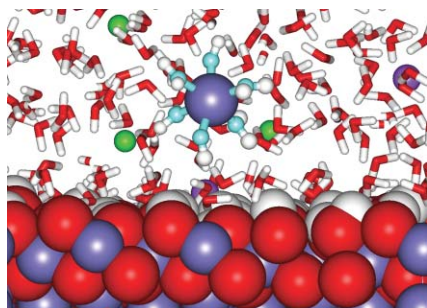
1989

**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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