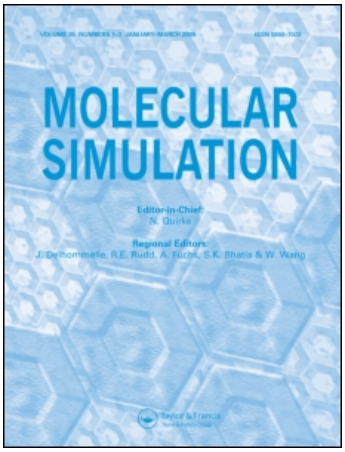

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Guest Editorial

M. Meunier

To cite this Article Meunier, M.(2008) 'Guest Editorial', Molecular Simulation, 34: 10, 887 — 888
To link to this Article: DOI: 10.1080/08927020802534850
URL: http://dx.doi.org/10.1080/08927020802534850

Molecular Simulation
Vol. 34, Nos. 10–15, September–December 2008, 887–888

Taylor & Francis
Taylor & Francis Group

Guest editorial

The present special issue of *Molecular Simulation* is a collection of over 50 papers, in which the modelling platform Materials Studio® (MS) was employed to build molecular models, run classical simulations or perform quantum mechanical calculations. MS package contains many different modelling approaches and this is reflected in the diversity of the articles presented here.

The first section of the issue contains papers related to *ab initio* calculations, using the density functional theory (DFT) method, and calculations performed at the semi-empirical level of theory. DFT, as implemented in the code DMol[3] seems to be a very popular package among MS users, as seen in the number of publications contained in the present edition of the journal. The second section of the issue contains papers related to classical simulations, where molecular dynamics is used to determine the properties of materials, for example, estimate mechanical properties of amorphous materials and predict materials compatibility. The third section contains papers using the Monte Carlo (GCMC) technique where adsorption isotherms in nanoporous materials are computed and the effect of the structure studied. The fourth section contains papers related to the area of crystallography where analytical instrument simulation tools were used to predict crystal structure or suspension stabilisation.

Materials Studio was first commercially released in June 2000, aiming to replace both Cerius[2] (of MSI) and InsightII (of Biosym) modelling platforms. The client (user interface) was made available under the Windows® operating system (as opposed to, for example, UNIX or Linux), thus giving access of the software to a wider group of people (at least at that time), in particular in the R&D departments of major chemicals companies [1]. Over the years, new modules were added so that modellers could use a diverse set of modelling and simulation techniques under one common interface. At the same time, the 'basic' functionalities, e.g. models building and visualisation, have also been subject to many improvements. Almost a decade later, MS contains a rather large list of about 25 modules, allowing the development of multi-scale modelling approaches required to tackle complex issues encountered in the chemical or pharmaceutical industries [2]. Current model building capabilities are also remarkable in letting users construct easily (i.e. from a simple-to-use interface) anything from multi-walled carbon nanotubes, dendrimers and heterogeneous systems, such as molecules and solvents on metal surfaces. Recent additions were made in the growing area of mesoscopic simulations. Such tools can be readily used for the study of complex fluids or predict the phase diagram of polymer blends, as well as their dynamical properties. In addition, a mesoscale molecule builder was included to create complex coarse-grained models that can be used in ordered configurations as an initial step of a simulation. MS also includes many codes taken from external collaborators or in collaboration with academics, e.g. CASTEP [3] or GULP [4]. Moreover, some of the recent developments originated from a nanotechnology consortium that has been running now for roughly 4 years, and has members ranging from major chemical companies to renowned academic institutions. New tools, including a linear scaling DFT application (ONETEP), a hybrid QM/MM application (QMERA) and a nanoparticle builder came out of the first phase of this consortium. Future developments will see the incorporation of a density functional tight-binding method (DFTB; http://www.dftb.org/) and a kinetic GCMC module into MS.

A scripting application program interface has been included recently to allow users to develop their own scripts inside MS. Users are able to automate tasks, perform customised analysis and integrate with other software. At the same time, some of the functionalities of MS have been integrated into a platform software called Pipeline Pilot [5]. Such tool allows users to develop their own protocols, or series of home-made tasks, calling any type of applications. Such tool permits full and easy integration of modelling software originating from various vendors. It also allows for scientific data generated from simulation or analytical instruments or else to be mined and analysed, and for reports to be generated in an automated fashion. It is still an open debate (http://accelrys.org/) whether the future of MS lies in more integration with such a productivity tool or continues to exist as a single molecular modelling environment with an ever-growing number of modules and functionalities, or both!

The number of papers presented here is too exhaustive to mention each one of them individually. However, it is noticeable that among the 54 selected papers, 26 come from the EMEA region, 11 from Asia Pacific and 17 from the Americas, demonstrating the global status of the MS

ISSN 0892-7022 print/ISSN 1029-0435 online

DOI: 10.1080/08927020802534850
http://www.informaworld.com

modelling package. Carbon nanotubes are still a very popular material to study, using modelling techniques. Properties investigated range from mechanicals to electronics. As mentioned earlier, DFT is the most reported modelling technique in this special issue. Such a tool has been increasingly reported in the rest of the scientific literature.

I would like to thank personally all the authors for their contributions, as well as all the referees for their support, and Prof. N. Quirke for reinviting me to be the guest editor of this special issue of *Molecular Simulation*.

M. Meunier
Cambridge, UK

References

M. Meunier, *Industrial applications of Molecular Simulation*, Special Issue of Mol. Simul. 32(2) (2006), pp. 71–72.

S. McGrother, G. Goldbeck-Wood, and M. Lam, *Integration of modelling at various length and time scales*, Lect. Notes Phys. 642 (2004), pp. 223–233.

M.D. Segall, P.J.D. Lindan, M.J. Probert, C.J. Pickard, P.J. Hasnip, S.J. Clark, and M.C. Payne, *First-principles simulation: ideas, illustrations and the castep code*, J. Phys.: Condens. Matter. 14 (2002), pp. 2717–2744.

J.D. Gale, *GULP – A computer program for the symmetry adapted simulation. of solids*, J. Chem. Soc., Faraday Trans. 93 (1997), pp. 629–637.

SciTegic (2008).