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Guest Editorial

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Guest Editorial – Special issue of Molecular Simulation on "*Industrial Applications of Molecular Simulation*"

The current special issue of *Molecular Simulation* presents many scientific papers related to the relevance of molecular modelling methods to industrial problems. Many modelling techniques are presented ranging from those based on quantum mechanics or so called ab initio methods to those using classical potentials and molecular dynamics. A wide range of materials are also studied in this issue from soft materials such as polymeric blends that are very widely employed in the chemical industry, to hard or inorganic materials such as glasses and alumina.

In the pharmaceutical research area, modelling and simulation have been extensively used over the last 30 years or so. Some large pharmaceutical companies have dedicated research centres for example in the context of drug discovery. However in materials science industries, the use of computational methods in general (and not only of modelling and simulations) is still novel, companies are equipped with intelligent databases and software packages based on statistical methods that can relatively quickly (and more or less accurately) estimate materials' properties. However the use of 'hard-core' modelling techniques (e.g. ab initio or other) in materials science is only growing slowly despite the recent steep increase in computer performance (required by such methods) and the low prices of high end supercomputers that should have allowed the spread of the modelling tools. One exception is academic research centres that have significantly benefited from these factors and are currently witnessing an increase in the use of modelling tools. In addition, the use of common operating systems to support such computer codes – that can be used for both productivity tools (e.g. e-mail) and for modelling codes – has contributed to the spread of the modelling techniques amongst materials scientists who may not be expert modeller. Furthermore, most recent commercial modelling software packages contain a wide range of techniques, the so-called 'integrated solutions', and today's modeller can easily access multiple techniques without having to swap from one vendor program and/or computer type to another. This in turn facilitates the development of the so-called 'multi-scale modelling[1] approach' that is so important for tackling problems as complex as those encountered in the chemical industry.

Thanks to all the advances in molecular modelling techniques, today's modeller can solve problems relevant to industry, and not just study a few clusters of atoms. Real materials in different conditions and formulations as well as important properties (e.g. polymer membranes and permeation as reported in this issue by D. Hofmann or P. Pullumbi) that can be compared to experimental data can nowadays be estimated relatively quickly, allowing the design of new materials (i.e. the so-called "Computer Assisted Molecular Design"). Macromolecular systems are routinely examined using methods based on classical potentials as demonstrated by the work of B. Derecskei on cellulose derivatives or on thermoplastic elastomers presented by J. Andzlem. Such large (amorphous) models can be studied with molecular modelling methods due to mathematical tricks like periodic boundary conditions; in addition, solvent conditions can be included in the models thanks to conductor-like screening model developed and reported here by B. Delley. Molecular modelling methods can also be employed to study complex inorganic materials using empirical pair potentials such as glass substrates as shown by S. Vyas or to estimate lattice energies and other thermodynamic properties of alumino silicates as exposed by V.L. Vinograd. Surface chemistry is a typical topic of study of methods based on quantum mechanics (e.g. Hartree-Fock, DFT, etc). The modelling tools allow the computation of adsorption energy to study for example metal

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deposition on alumina surface shown by A. Chatterjee. Simplified ab initio methods, such as the so-called semi-empirical methods (e.g. MNDO, AM1, etc) exist that are computationally less demanding without a great loss of accuracy. In this special issue such methods were employed by M. Plummer to study the decomposition mechanism of hydrogen sulphide, which is relevant to the petrochemical industry. At last but not least, methods based on structure-activity relationship where empirical correlations are drawn between the chemical structure of the models and their activity that are so commonly used in the pharmaceutical area are now finding their way into the 'chemical' world. An example of the use of such a tool for the computation of thermodynamics data of oxygen-containing heterocycles is described in this special issue by N. Adams.

The rise of research funding in the Nanotechnology area (and in particular in the nanobiology field) is encouraging the development of modelling techniques as these methods are well suited for studying problems (or materials) at the nanoscale. Additionally, the use of 'materials' techniques in the (bio)-pharmaceutical sector to study e.g. drug preformulation and drug delivery systems is also contributing to the spread of such tools in the industrial arena.

The cost of having a modeller inside a company today does not resides anymore in the cost of both hardware and software but mostly in the cost of labour. In such a context, one may wonder why the number of materials modellers in the chemical industry is still relatively low (e.g. compared to synthetic chemists). Is it a lack of expert modellers and thus an opportunity for new graduates as mentioned by J.M. Newsam[2] or is it that modelling and simulation are still regarded by the chemical industries as an academic solution despite all the recent developments in the field and the numerous 'case studies' where modelling techniques have been used successfully to solve problems of industrial importance? Could it be simply a matter of lack of publicity or marketing that the industry does not yet know the full potential of such computational tools? The fact that nowadays most science graduates in chemistry or related subjects have at some stage during their studies been introduced to molecular modelling will surely make the spread of such techniques in the industrial chemical world easier in the near future.

I do hope that such a special issue of *Molecular Simulation* will contribute to the introduction of molecular modelling techniques in the ever challenging area of materials science in the industrial world and would like to thanks personally all the authors for their contribution and N. Quirke for his trust (and patience!) in inviting me to be guest editor of this journal.

M. Meunier
Cambridge, U.K. 2006

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1 S. McGrother, G. Goldbeck-Wood, and Y.M. Lam, Integration of Modelling at Various Length and Time Scales, Lecture Notes Phys. 642, 223–233 (2004).
2 J. M. Newsam, Foreword of *Molecular modelling techniques in materials science,* JR Hill, L. Subramanian and A. Maiti. CRC Press (2005).

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