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## Guest Editorial

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## Guest Editorial

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3 Guest Editorial – Special issue of *Molecular Simulation* on “*Industrial Applications of*  
4 *Molecular Simulation*”  
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8 The current special issue of *Molecular Simulation* presents many scientific papers related to  
9 the relevance of molecular modelling methods to industrial problems. Many modelling  
10 techniques are presented ranging from those based on quantum mechanics or so called ab  
11 initio methods to those using classical potentials and molecular dynamics. A wide range of  
12 materials are also studied in this issue from soft materials such as polymeric blends that are  
13 very widely employed in the chemical industry, to hard or inorganic materials such as glasses  
14 and alumina.  
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17 In the pharmaceutical research area, modelling and simulation have been extensively used  
18 over the last 30 years or so. Some large pharmaceutical companies have dedicated research  
19 centres for example in the context of drug discovery. However in materials science industries,  
20 the use of computational methods in general (and not only of modelling and simulations) is  
21 still novel, companies are equipped with intelligent databases and software packages based on  
22 statistical methods that can relatively quickly (and more or less accurately) estimate materials’  
23 properties. However the use of ‘hard-core’ modelling techniques (e.g. ab initio or other) in  
24 materials science is only growing slowly despite the recent steep increase in computer  
25 performance (required by such methods) and the low prices of high end supercomputers that  
26 should have allowed the spread of the modelling tools. One exception is academic research  
27 centres that have significantly benefited from these factors and are currently witnessing an  
28 increase in the use of modelling tools. In addition, the use of common operating systems to  
29 support such computer codes – that can be used for both productivity tools (e.g. e-mail) and  
30 for modelling codes – has contributed to the spread of the modelling techniques amongst  
31 materials scientists who may not be expert modeller. Furthermore, most recent commercial  
32 modelling software packages contain a wide range of techniques, the so-called ‘integrated  
33 solutions’, and today’s modeller can easily access multiple techniques without having to swap  
34 from one vendor program and/or computer type to another. This in turn facilitates the  
35 development of the so-called ‘multi-scale modelling<sup>1</sup>’ approach’ that is so important for  
36 tackling problems as complex as those encountered in the chemical industry.  
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42 Thanks to all the advances in molecular modelling techniques, today’s modeller can solve  
43 problems relevant to industry, and not just study a few clusters of atoms. Real materials in  
44 different conditions and formulations as well as important properties (e.g. polymer  
45 membranes and permeation as reported in this issue by D. Hofmann or P. Pullumbi) that can  
46 be compared to experimental data can nowadays be estimated relatively quickly, allowing the  
47 design of new materials (i.e. the so-called “Computer Assisted Molecular Design”).  
48 Macromolecular systems are routinely examined using methods based on classical potentials  
49 as demonstrated by the work of B. Derecskei on cellulose derivatives or on thermoplastic  
50 elastomers presented by J. Andzlem. Such large (amorphous) models can be studied with  
51 molecular modelling methods due to mathematical tricks like periodic boundary conditions;  
52 in addition, solvent conditions can be included in the models thanks to conductor-like  
53 screening model developed and reported here by B. Delley. Molecular modelling methods can  
54 also be employed to study complex inorganic materials using empirical pair potentials such as  
55 glass substrates as shown by S. Vyas or to estimate lattice energies and other thermodynamic  
56 properties of alumino silicates as exposed by V.L. Vinograd. Surface chemistry is a typical  
57 topic of study of methods based on quantum mechanics (e.g. Hartree-Fock, DFT, etc). The  
58 modelling tools allow the computation of adsorption energy to study for example metal  
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3 deposition on alumina surface shown by A. Chatterjee. Simplified ab initio methods, such as  
4 the so-called semi-empirical methods (e.g. MNDO, AM1, etc) exist that are computationally  
5 less demanding without a great loss of accuracy. In this special issue such methods were  
6 employed by M. Plummer to study the decomposition mechanism of hydrogen sulphide,  
7 which is relevant to the petrochemical industry. At last but not least, methods based on  
8 structure-activity relationship where empirical correlations are drawn between the chemical  
9 structure of the models and their activity that are so commonly used in the pharmaceutical  
10 area are now finding their way into the 'chemical' world. An example of the use of such a tool  
11 for the computation of thermodynamics data of oxygen-containing heterocycles is described  
12 in this special issue by N. Adams.

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

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

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

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45 M. Meunier  
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