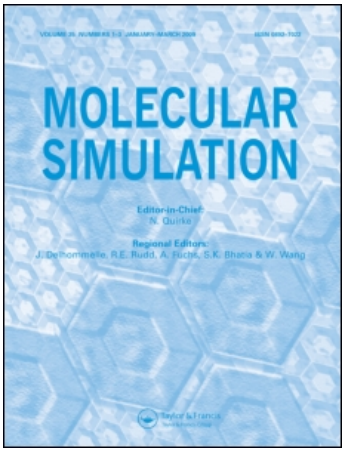

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Editorial

N. Quirke

To cite this Article Quirke, N.(1989) 'Editorial', Molecular Simulation, 2: 4, i — ii
To link to this Article: DOI: 10.1080/08927028908034602
URL: http://dx.doi.org/10.1080/08927028908034602

Molecular Simulation, 1989, Vol. 2, pp. i–ii
Reprints available directly from the publisher
Photocopying permitted by license only

EDITORIAL

It is twenty four years since the publication of Anees Rahman's paper on the molecular dynamics of argon. An event which can now be seen to have greatly enlarged the ambitions of computational statistical mechanicians to include the simulation of "real" systems. During the last quarter century molecular simulation methods have been applied to a great variety of ever more complex materials many of which are of industrial significance. In recognition of the growing importance of simulation to industry, in January 1988 the annual conference of the UK Science and Engineering Research Council's Collaborative Computational Project 5, better known as CCP5, held at Birkbeck College, University of London was devoted to the topic of Industrial Applications of Molecular Simulation. The conference organisers were Professor C.R.A. Catlow (University of Keele) and Dr. N. Quirke (British Petroleum). Some fifty papers and posters were presented on applications ranging from the phase and rheological behaviour of dense fluids to the properties of ceramic materials. A selection of the papers presented at the meeting form the present issues of *Molecular Simulation*. The conference was a resounding success with over 130 scientists attending representing Universities, Polytechnics, goverment research laboratories and industrial research centres in Europe, North America and China. The meeting opened with an introductory lecture by Dr. N. Quirke setting out the role of molecular simulation in an industrial research centre. The scientific programme was divided into eight sessions concerned with the use of molecular simulation to help solve important problems in the areas of a) bulk fluids b) solid state chemistry c) macromolecules d) biological materials e) materials (three sessions) and f) porous media. (For the purposes of these proceedings the papers have been grouped into three sections – (i) simulation of bulk fluid properties and (ii) simulation of fluids in pores, both published as Issues 2(4–6) of *Molecular Simulation*, and (iii) simulation of materials (iii), published as Issues 3(1–3) of *Molecular Simulation*.)

Several major themes emerged from the conference which are reflected in these proceedings. A number of speakers dealt with the use of molecular simulation to provide exact data for simple model systems against which theories could be unambiguously tested. Such models tend to be idealised representations of real fluids which nevertheless contain the essential physics of the problem. This use of molecular simulation is of particular help in the formulation of improved theories of liquids which may lead to better equations of state and scaling laws for physical property predictions – a problem of immense industrial importance. The use of simplified models can be of great benefit when trying to understand phenomena in heterogeneous or disordered substances such as those sometimes used as adsorbents or catalyst supports. Experiments on these systems will usually yield results which represent averages over many microscopic environments (e.g. pore widths or impurity concentrations). Molecular simulation on the other hand can provide detailed results (e.g. diffusion coefficients or adsorbtion properties) for well defined local structures. In this way although it will not be possible to simulate the whole material, key phenomena may be isolated and related to specific microstructures.

The greatest number of papers dealt with the challenging task of constructing and simulating realistic models of industrially important materials including catalysts,

ceramics, glasses, solid electrolytes, biologically important macromolecules, polymers, photographic, electro-optic and laser host materials. One of the goals of this work is to produce a sufficiently reliable model of the real system that information on microscopic events (often experimentally difficult or impossible to observe) may be obtained and used to design, at the molecular level, new processes and materials. For these purposes the great strength of molecular simulation is the ease with which changes may be made to the models (such as substituting one metal ion for another) and the consequences observed. Systems which might require months of experimental effort to synthesise can be constructed on the computer and their properties predicted within hours.

The papers in these proceedings make it very clear that molecular simulation is an attractive research tool in the study of industrially relevant problems. It is however true that some applications are presently circumscribed by the lack of fast convenient methods of calculating potential energy surfaces, indeed for many problems and especially those which involve chemisorption, it is not possible to discuss molecular simulation in isolation from quantum mechanics. A number of new approaches are currently under development which seek to integrate the two; a first step being the straightforward combination of molecular simulation with *ab initio* methods.

Molecular simulation is now an important part of a battery of theoretical techniques including quantum chemical methods and phenomenological models (e.g. structure-property relationships) which are changing the way new industrial processes and materials are developed.

N. Quirke.