Statistical Mechanics and Thermodynamics Group

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ANNUAL REPORT 1998

Membership

The membership of the Group on 11/12/98 stood at 154.

Committee

The committee until the AGM for 1999 consists of:

Chair Prof. M.P. Allen (Bristol)

Hon. Secretary Dr. D.J. Cleaver (Sheffield Hallam)

Hon. Treasurer Dr. P.D. Olmsted (Leeds)

Ordinary Members: Dr. S. Goodwin (BP, Sunbury)

Prof. J.-P. Hansen (Cambridge) Dr. P.G. Higgs (Manchester)

Dr. J. Jones (Unilever, Port Sunlight)
Dr. P. Warren (Unilever, Port Sunlight)

Dr. R. Wheatley (Nottingham)

Meetings and other activities during 1998

Early in the year, we supported the established CCP5 Spring School on *Methods in Molecular Simulation* run by Profs. M.P. Allen and D.J. Tildesley in Bristol, March 24-31. Immediately following this, and in the same venue, the group ran a one day workshop on *Classical Density Functional Theory*, the principal lecturer being Prof. R. Evans. On June 22, the Group held a one-day meeting in Manchester entitled *Novel Applications of Statistical Mechanics*. This was held in collaboration with the Theoretical Condensed Matter Physics group of the IOP, the theme being applications of statistical mechanics outside of traditional physics and chemistry. The Group's AGM, was incorporated into this Manchester meeting.

Completed 1999 Events and Future plans

Our first event for 1999 was a one-day workshop "An Introduction to the Fundamental Concepts of Polymer Dynamics" led by Prof. Tom McLeish. This took place on 7 January at the Leeds Polymer IRC. The SMTG has two main meetings planned for 1999. The first, entitled "Interactions, Phases and Flow of Colloids", a joint workshop of the Soft Matter and Liquids Networks held in conjunction with ourselves, will run from 29 - 31 March at Cambridge University. It will be devoted to the static and dynamic aspects of colloidal dispersions and will incorporate the group AGM. The second meeting, "Biomolecular Folding and Self Assembly" will run from 12-14 April at Salford University as part of the IOP's annual congress. It will address the structure and folding mechanisms of biological macromolecules, including proteins, nucleic acids, polysaccharides and lipids, and the self-assembly of these molecules into larger scale structures. This meeting will incorporate the 1999 Lennard-Jones Lecture: "Regulation of Cellular Processes by the Membrane-Bending-Elasticity Concept", delivered by Prof. E. Sackmann (Garching).

This year's "Methods in Molecular Simulation Summer School" will be held at UMIST from 21 - 29 June. The principal lecturers will be Profs. J.H.R. Clarke (UMIST), M.P Allen (Bristol), and D.J. Tildesley (Unilever) with Dr W. Smith (Daresbury) and support will come from CCP5, the ESF network SIMU and Unilever as well os our group. Again, we shall follow the school with a one-day workshop, this one being on "Mesoscale Modelling". Principal lecturers will be Drs. M. Haagen (Unilever), N. Spenley (Unilever) and J. Yeomans (Oxford). The intention here is to give an introduction to, and overview of, the use of Lattice Boltzmann and Dissipative Particle Dynamics methods for the simulation of fluids in bulk and restricted geometries. A further one-day workshop may follow later in the year, but dates and venues have yet to be established.

Accounts

The accounts for the year 1998, prepared by the (now retired) Hon. Treasurer Dr. A.J. Masters, are attached herewith.

D.J. Cleaver (Sheffield Hallam) Hon. Sec.