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PREFACE

This Special Issue contains contributions to the Euroconference Dynamics of Complex Molecular Systems - Computer Simulations and Experiments, held at Vaalsbroek (The Netherlands) from May 24th to 28th, 1998. It was the last one in a series of four Euroconferences within the conference programme Technical Advances in Particle-Based Computational Materials' Sciences, financed by the European Union. The conference brought together scientists studying macromolecules and complex liquids by experimental techniques and computer simulations. The aim of the meeting was to promote a combined approach of experiments and simulation.

It is now more and more recognised that the experimental studies of liquids and macromolecules by NMR, neutron scattering and other spectroscopic techniques yield an enormous amount of information, which is a priori difficult to interpret in terms of simple models. This does not mean that certain aspects of such so-called complex systems cannot be described by simple models, but that the decision which model describes reality is ambiguous since different models may fit the data equally well. Here computer simulations play an important role since they give access to even more details about a system than experiments, provided that the simulations are validated by the experimental data. Using sophisticated algorithms and powerful computers allows us nowadays to perform realistic studies of complex molecules and liquids and to compare the results to experimental data on a semi-quantitative or even quantitative basis. There is a particular need to understand the microscopic dynamics of biomolecular systems, for example aspects of slow dynamics and hydration. Knowledge about the essential features of the energy landscape of proteins and peptides is still very limited in spite of the vast amount of available experimental data related to this subject. Therefore it is not surprising that most contributions to this Special Issue focus on biological systems; however, there was also a strong component of oral contributions and posters concerning other systems, especially liquid crystals.

We would like to thank all participants and invited lecturers for their contributions to the conference and to this issue, and we acknowledge the financial support of the European Science Foundation, which made this meeting possible. It is a special pleasure for us to thank Michel Mareschal (Université Libre de Bruxelles) and Manfred Zeitler (RWTH Aachen) for helping us to organise this meeting.

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