New trends in simulating colloids and self-assembling systems

2010 J. Phys.: Condens. Matter 22 100301

(http://iopscience.iop.org/0953-8984/22/10/100301)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER
J. Phys.: Condens. Matter **22** (2010) 100301 (2pp) doi:10.1088/0953-8984/22/10/100301

INTRODUCTION

New trends in simulating colloids and self-assembling systems

Guest Editors

Giuseppe Foffi
Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Gerhard Kahl
Vienna Technical University, Austria

Interest in colloidal physics has grown at an incredible pace over the past few decades. To a great extent this remarkable development is due to the fact that colloidal systems are highly relevant in everyday applications as well as in basic research.

On the one hand, colloids are ubiquitous in our daily lives and a deeper understanding of their physical properties is therefore highly relevant in applied areas ranging from biomedicine over food sciences to technology. On the other hand, a seemingly unlimited freedom in designing colloidal particles with desired properties in combination with new, low-cost experimental techniques, make them—compared to hard matter systems—considerably more attractive for a wide range of basic investigations. All these investigations are carried out with close cooperation between experimentalists, theoreticians and simulators, reuniting thereby, on a highly interdisciplinary level, physicists, chemists, and biologists.

In an effort to give credit to some of these new developments in colloidal physics, two proposals for workshops were submitted independently to CECAM in the fall of 2008; both of them were approved and organized as consecutive events. This decision undoubtedly had many practical and organizational advantages. Furthermore, and from the scientific point of view more relevant, the organizers could welcome in total 69 participants, presenting 42 oral and 21 poster contributions. We are proud to say that nearly all the colleagues that we contacted at submission time accepted our invitation, and we are happy to say that the number of additional participants was rather high. Due to the fact that both workshops took place within one week, quite a few participants, registered originally for one of these meetings, extended their participation to the other event also. In total, 23 contributions have been submitted to this special issue, which cover the main scientific topics addressed in these workshops. We consider this relatively high number of contributions as an indicator that the topics presented at these workshops represent substantial scientific developments.

The particular motivation to organize these two workshops came from the fact that experimental work in colloidal physics is advancing rapidly around the globe. In contrast, theoretical and simulation approaches to investigate the wide range of new and surprising physical phenomena of colloidal systems is lagging behind this experimental progress. This is the more deploring since theory and simulation might provide a more profound understanding of many phenomena in soft and bio-related physics, such as phase behaviour, self-assembly strategies, or rheological properties, to name but a few. Furthermore this insight might help to guide experiment to design new colloid-based materials with desired properties. The declared aim of the two workshops was thus to bring together scientists who have contributed in recent time to new developments in colloidal physics and to share and discuss their latest innovations.

While CECAM workshops traditionally bring together scientists from the theoretical and simulator communities, from the very beginning the organizers considered it an indispensable necessity to invite experimentalists. And indeed, the organizers are happy to confirm that the participation of experimentalists, theoreticians, and simulators was highly fruitful and mutually inspiring:

discussions between all communities did help to understand the possibilities and limitations imposed by experiment, theory, and simulations. Reuniting thus all forces, the workshop did contribute to a deeper understanding in colloidal physics and has helped to address future aspects that might lead to more applied problems of technological relevance.

The first workshop, entitled 'Computer Simulation Approaches to Study Self-Assembly: From Patchy Nano-Colloids to Virus Capsides', (organized by Jonathan Doye—University Of Oxford, Ard A Louis—University Of Oxford and Athanassios Panagiotopoulos—University Of Princeton) focused on the remarkable ability of colloidal systems to self-organize in well-defined composite objects. New simulation techniques and theoretical approaches were presented and discussed that offer a deeper understanding of self-assembly phenomena in colloidal physics and, eventually to uncover design rules for self-assembly. Particular emphasis was put on an emerging new class of colloidal particles, so-called patchy colloids. The second workshop, entitled 'New Trends in Simulating Colloids: From Models to Applications', (organized by Giuseppe Foffi—Ecole Polytechnique Fédérale De Lausanne, Gerhard Kahl—Vienna Technical University and Richard Vink—Georg-August-Universität Göttingen) focused on new methodological devices in theoretical and simulation approaches that provided a more profound insight in colloidal physics in general. A large variety of theoretical tools, ranging from different simulation techniques over classical density functional theory to efficient optimization techniques were presented. For details about the tools presented in both workshops we refer the reader to the contributions of this special issue. The 'round table' discussion meetings were highly useful in providing an overview of yet unsolved problems and to point out directions for future work. From the phenomenological point of view, among those are the question on the relevance of hydrodynamic interactions, the problem whether to treat solvents in an explicit or implicit way, or the relevance of multibody interactions, to name but a few. With respect to the methods it was agreed that future developments on dynamic Monte Carlo simulations or on rare events and multiscale techniques are urgently required. The presence of the experimentalists was also of great help in focusing attention on the systems that are going to represent the scientific challenges in the next years. It was interesting that while new materials like dna-coated colloids or janus and patchy particles are generating a lot of interest, more traditional systems, like colloidal glasses/gels and proteins, are far from being completely understood.

The relevance of these two workshops was reflected by the general consent that within a few years' time events with similar aims should be organized to discuss the progress that has been achieved.