Report for the Cecam workshop "Simulations of Novel Carbon Materials"
held at CECAM in Lyon, France
25th to 28th of October 2006

Background

Carbon continues to reveal new surprises and the workshop showed that the research in carbon is as vital as fifteen years ago, when the nanotube were (re)discovered. There exist a number of conferences devoted to Carbon materials, like the Carbon-conferences and the NT-series. However, the theoreticians are a minority at these conferences and it is necessary to have a workshop dedicated to the theoretical treatment of carbon materials. The focus of the workshop, dedicated to simulations of carbon materials, was therefore highly appreciated.

The format of the workshop

The workshop was divided into 20 lecture by invited speakers, a poster presentation and two poster sessions with food, and finally a summary and discussion. The schedule for the talks was divided into 45 minutes slots. Each timeslot for a talk had 30 minutes devoted to the talk and 15 minutes discussion, which was a successful concept. Every talk provoked a lively discussion and the 15 minutes assigned after each talk was long enough to allow for a sufficient discussion. The 15 minutes allocated for discussion also worked as buffer to keep the time schedule.
The final summary was made by the young participants. This gave a very good overview of the workshop from a new perspective. The final discussion, organized as a round of comments where every participant got the opportunity to say their opinion, was very informative.

The location for the Workshop

CECAM is a very good site for this kind of workshop. The secretaries Emmanuelle Crespeau and Emilie Bernard are helpful to organize the practical arrangement with such things as hotel bookings, poster boards and catering. CECAM has good infrastructure with the conference room, area for poster session and the coffee breaks in close proximity. The projector for power-point presentation and w-LAN worked very well.

Subjects covered during the Workshop

The contributions covered a large number of different carbon materials, ranging from the established forms of carbon like graphene and nanotubes to newly proposed structures as carbon foams and clathrates. This indicates that there may still be more forms of carbon materials to be discovered. Theory may here play a vital role in order to predict new structures and to evaluate the properties of hypothetical structures that may not easily be generated in the laboratory.
A number of different aspects were discussed along these lines, like the phase diagram, the growth of nanotubes, the influence of defects, magnetic, transport and chemical properties of carbon materials.

Methods discussed during the Workshop

A number of different methods were used to model and simulate this diverse range of properties. Ab-initio methods, tight-binding and empirical potentials were used together with thermodynamics, Monte Carlo techniques and molecular dynamics. The workshop brought the two communities that are using ab-initio methods and empirical potentials together. There were lively discussions about the range of applicability of the different methods. The empirical potentials on one hand have the

advantage of being faster and the possibility to include long-range interactions that are important for graphitic systems. However, the workshop showed that designing a good empirical, transferable, potential is a difficult task. For instance, five different empirical potentials for carbon were presented. Ab-initio methods on the other hand are more accurate for the interatomic interaction, but there is still a need for an exchange-correlation functional that include van-der Waals interaction.

Scientific outcome
The lectures had a very high quality and initiated lively discussions that continued during coffee breaks and the poster sessions. A number of potential collaborations were initiated between the participants. It was decided to make a comparison between the five empirical potentials that were presented in order to evaluate their quality. It was also discussed to form a network for simulations of carbon materials.

Recommendations
There is a need for a workshop devoted to simulations and modeling of carbon materials. It was suggested that a similar workshop should be organized in two years.

The format of the workshop was successful: 45 minutes slots for the talks with 30 minutes talk and 15 minutes discussion. The workshop also included a poster session where food and drinks were served. This format could also be used for the next workshop.

A network for simulations of carbon materials should be formed. One of the tasks would then be to maintain this workshop as a continuing event.

It was suggested that next workshop, in addition, should have a few keynote lectures from experimentalists. These lectures should point out some important problems where theory and modeling would be particularly useful to solve an important problem.

On the behalf of the Organizers

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