

Report on CCP5 Sponsored Visit to the United Kingdom (June 22 - 30 1998)

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My tour of UK Universities has been through Cambridge, Bristol and Daresbury Laboratory.

In Cambridge I have been in touch mostly with the group of Prof. J.-P.Hansen in the Chemistry Department. We have discussed about current issues in the classical density functional treatment of charged systems, which he has been studying for some years. Interesting insights and possibilities for collaboration on biophysical systems have emerged. In view of my permanence in Cambridge in his group starting next September, we have discussed a research project about the influence of electrostatics in structural and kinetic properties of ionic channels. Discussions with post-doctoral students of that group, namely with Dr. David Goulding and Dr. Ard Luiss, who are involved in projects concerning electrostatics and statistical properties of polymers, have been a very useful source of scientific sharings. I have discussed also with Prof. Michiel Sprik, who is working on ab-initio simulations of molecules and who is interested in efficient sampling and detection of intermediate states of chemically reactive systems. A possible collaboration is in view on some specific reactive systems. In the chemistry department I have given a talk on some recent results on the glass-like transition of proteins, as revealed by molecular dynamics studies. Subsequent feed-back with the audience has been a very useful occasion to discuss on this issue.

In Bristol I have been hosted by Prof. M. Allen of the Physics Department. Prof. Allen's main interest is in liquid crystals. Although our research fields are different he has a long experience in molecular dynamics simulation techniques. Conversations on recent developments in this field have been very interesting. Also our meeting has been the occasion to share scientific software. I have also discussed with a post-doctoral student of his group, Dr. Guido Germano, on recent advances in liquid crystals and molecular dynamics. In Bristol a very useful discussion has been with Prof. G. W. Neilson, and we have shared some results on biological systems, as he has recently performed neutron scattering experiments on polypeptides. The talk in Bristol, regarding the same subject as in Cambridge, has been an important source of discussion and insights.

In Daresbury I have been hosted by Dr. W.Smith and I had a very fruitful discussion on molecular dynamics, both as a technique and applications to complex systems. The future of the MD codes that we are developing independently (DL_POLY and DLPROTEIN) has been discussed and loosely planned. Sharing of software of this kind has also been very important. In Daresbury I had important discussions with Dr. Nic Harrison, about ab-initio simulation of systems in the crystal phase, with Dr. Phil Lindan, on simulation of systems modeled with dynamic polarizability, and briefly with Dr. Maurice Leslie. I am very grateful to Dr. James Nicholson for an instructive tour of the Synchrotron.

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