

# MINUTES OF THE CCP3 WORKING GROUP MEETING

Daresbury Laboratory

Wednesday 17<sup>th</sup> April

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Present	Apologies
Dr. AJ Fisher (chair)	Dr. JF Annett
Prof. J. Inglesfield	Prof. D Bird
Dr. S Crampin	Dr. J Blackman
Prof. G Thornton	Dr. P Durham
Prof. NM Harrison	Dr. M Finnis
Dr. J Purton	Prof. W Flavell
Dr. BG Searle	Prof. R Godby
Dr. GP Srivastava	Dr. S Holloway
Prof. G Thornton	Dr. R Lambert
	Dr WC Mackrodt
	Prof. J A D Matthew
	Prof. D Norman
	Dr. C Norris
	Dr. RE Palmer
	Dr. S Parker
	Prof. JB Pendry
	Dr. P Rous
	Prof. R Smith
	Dr. S Tear
	Dr. T. Turner
	Dr. A Wander
	Prof. P Weightman
	Prof. DP Woodruff

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## Apologies for absence

Apologies for absence were noted.

## Minutes of the previous meeting (05/04/2001)

The minutes were approved as an accurate record of the last meeting.

# Matters Arising

## Possible Collaboration and Meetings with CCP5

AF and John Harding had discussed several possible areas in which CCP5 (molecular simulation) and CCP3 might collaborate. These are:

- Mesoscale surface structure. Possible meeting for 2004.
- Combined simulations of scattering and surface dynamics.
- Building and simulating nanostructures. A possible meeting with the UCL based IRC in Nanotechnology

The WG was very supportive of these suggestions and AF was encouraged to pursue the possibilities further.

**Action: AF**

## Membership of the Working Group

The working group accepted the resignation of Tracey Turner as member and wished to thank her for all of her efforts in support of CCP3 over many years.

Dr John Purton (soft X-ray group, Daresbury Laboratory) was elected as a member of the working group.

## Flagship grant - status report

JI and BGS presented information about the recently funded flagship grant - "Development of New Methodologies for the Interpretation of X-ray Absorption Spectra", GR/R68542/01. The grant has a formal start date of 01/04/2002 and provides for a PDRA based at Daresbury; interviews for this position will be held on 26/04/2002. The work plan consists of a number of updates to the EXCURV software (including its interface to DLV2.1) to be followed by the development of a full potential, self-consistent code for predicting X-ray absorption.

The grant covers CCP3's T&S expenditure for the next 3 years. The meeting commended the hard work of Adrian Wander as the main instigator and author of the grant.

# Report on the CCP Steering Panel Meeting

AF gave an oral report on the recent CCP steering panel meeting which is summarised below.

- Prof. Mike Allan has offered to step down as chair of the steering panel but would stay on if re-elected.
- The joint CCP bid to the eScience programme has been rejected. The main objections cited were that the bid was concerned with science rather than eScience and that it was too broad in its scope. Efforts are being made to identify alternative funding for this proposal.
- The EPSRC have decided that future CCP funding will be split into *network grants*, which cover the activities of the working group, workshops and visitors, and *flagship grants*, which will be submitted in responsive mode and provide resources for the development of new functionality and scientific projects.

Within this new scheme any given CCP can submit several flagship grants. The WG decided that the previously unfunded grant aimed at studying metal clusters on oxide surfaces, which was very favourably reviewed, should be resubmitted.

**Action: NMH,JB,MF,RS**

The working group considered a number of new potential areas of interest and decided that two in particular could be pursued.

- A localised basis set formalism for the calculation of STM spectra. One of the main aims of the new code would be to interpret low temperature, single molecule, vibrational data for which experimental facilities are being developed in Manchester. This formalism may also be useful for interpreting data from the XPEEM experiment planned for the DIAMOND facility.

**Action: GT,AF**

- The exploitation of the ability to compute phonon frequencies and eigenvectors in order to improve the interpretation of IR, HREELS, RAMAN measurements and improve the models of thermal averaging used in the current interpretation of SXRD, XPS, ARUPS and EXAFS spectra. This project might be integrated with the planned developments of a free electron laser for IR-spectroscopy at Daresbury.

**Action: GPS,NMH**

Those actioned in each of these areas will produce a report at the next WG meeting on progress in developing a flagship proposal.

## **DLV Status Report**

BGS presented details of the latest released of DLV (version 2.1) which is now available for downloading from the DLV web site - <http://www.cse.dl.ac.uk/Activity/DLV>. The code provides for the visualisation and editing of bulk and surface structures and a full interface to CRYSTAL-98 calculations (setting up calculations, remote job hosting, analysis of properties etc.). It runs on a wide variety of Unix and Windows machines. About 20 groups have copies of the code already. The next stage is to introduce the ability to model semi-infinite surfaces so that surface modelling codes with the CCP3 library can be interfaced conveniently.

WG members were encouraged to ensure that their research groups downloaded a copy and provided BGS with feedback and suggestions.

## **Visitor Programme**

The following visitors were proposed and accepted the working group.

Dr R. Miotto (San Paolo, Brazil), and Dr Tutuncu (Canada) , to visit GPS in Exeter.

Dr D. Munoz (University of Barcelona) to visit Imperial, Daresbury and UCL.

JI noted that Dr JM Pitarke (“lifetime of electronic states at surfaces”) and Dr Hiroshi Ishida (“Embedding methods”) would be visiting his group for 6 months from Sept. 2002.

## **Workshops**

The CCP3 code training day in November 2001 was a great success; the WG confirmed that, if practical, this should be an annual event. The possibility of future training days in combination with other CCP’s or SRRTNet should be explored.

**Action: AW,BGS,NMH**