

# MINUTES OF THE CCP3 WORKING GROUP MEETING

University College London

---

Present	Apologies
Dr. AJ Fisher (chair)	Prof. W Flavell
Dr. A Wander	Dr. P Durham
Dr. BG Searle	Prof. NM Harrison
Prof. G Thornton	Dr. J Purton
Dr. S Tomic	Dr. J Blackman
Prof. G Thornton	Prof. R Godby
Prof. GP Srivastava	Prof. DP Woodruff
Dr M Warren	Dr EA Colbourn
Prof. R Smith	Prof. M Finnis
	Prof. D Bird
	Dr. S Holloway
	Dr. R Lambert
	Dr WC Mackrodt
	Prof. J. Inglesfield
	Dr. S Crampin
	Prof. J A D Matthew
	Prof. C Norris
	Dr. S Parker
	Dr S Tear
	Prof. P Weightman
	Dr. W Hofer
	Prof. Sir JB Pendry

---

## 1 Apologies for absence

Apologies for absence were noted.

## 2 Minutes of the previous meeting (22/07/2004)

The draft minutes had the location of the meeting as DL. This meeting was in fact held at UCL. With that correction the minutes were approved as an accurate record of the last meeting.

**Action: AW to correct and install on web**

## 3 Matters Arising

### 3.1 DIAMOND Interactions

AJF has contacted PJD in connection with CCP3/DIAMOND interactions. Discussions are in progress.

**Action: AJF to continue discussions**

### 3.2 Non-linear Optics

This action should be deleted.

### 3.3 Visitor Reports

AW has not yet received reports on visitors from NMH, GPS, JI and SC.

**Action: NMH, GPS, JI and SC to provide short reports to AW  
asap**

### 3.4 Visitors

The proposed visit from the Russian visitor was discussed. This may still go ahead. Lev Kantarovich is interested in this area and needs to be consulted

**Action: AJF to discuss visitors with LK**

It was suggested that LK should be invited to join the committee

**Action: AJF to invite LK to join the working group**

## 4 Grant Updates

### 4.1 Single Molecule Spectroscopy Grant

AJF reported on the status of this grant which has been submitted and contains the infrastructure money for CCP3 from Jan 2006.

### 4.2 Clusters Grant

In the absence of NMH and MF detailed discussion of this grant was postponed until the next meeting.

**Action: NMH and MF to report to the next meeting**

The meeting discussed a number of possible themes for future flagship grants. In a number of cases we would need to organise workshops before proceeding with such grants;

### 4.3 Dynamics and Excited States

It was felt that there may be scope for a workshop in this area.

**Action: AW and RG to investigate and report to the next meeting**

### 4.4 Magnetic Properties of Surfaces

AJF reported on discussions with James Annett. There is scope for a joint workshop in this area. It was suggested that WH might wish to organise this meeting. If not, it was suggested that the meeting could be held at DL with AW and Walter Temmerman organising.

**Action: AJF to contact James Annett to identify CCP9 organiser and liase with WH**

### 4.5 EXAFS

It was felt that possible continuation of the current EXAFS project should be left to CCLRC and probably was not suitable for a further grant submission. The key science driver identified by the community has been addressed by the current grant and the long term maintenance of the code is probably best handled by CSED/SRD/DIAMOND.

### 4.6 CCP5 Interactions

The possibility of a flagship grant concerning wet (mineral) surfaces or large (chiral) organic molecules at surfaces was also discussed. There is clear overlap in these areas with CCP5 and the meeting felt that a joint CCP3/CCP5 workshop in one of these areas should be held.

**Action: AJF to liase with John Harding on possible theme of a workshop. MW volunteered to organise if the theme was minerals.**

## 4.7 Semiconductor Surfaces and Quantum Dots

This area does not currently fall within the remit of any of the CCP's. It was felt that this issue should be considered by the CCP steering panel.

**Action: AJF to raise at next steering panel meeting**

In preparation for possible future grant submissions we need to update the publications lists, visitor lists and workshop lists.

**Action: ALL submit updated lists to AW. The current publication list is available via <http://www.ccp3.uk/Coordination/CCP3/pubs.htm>**

## 5 CCP3 HPCx Bid

PWo, MW, AJF, WH, GPS and AW plan to submit a consortium bid for HPCx time. If any other members of the working group would like to contribute to this request please contact AW as soon as possible.

## 6 Hector

AJF has been contacted by Hugh Piltcher-Clayton and asked to comment on the Hector procurement. The meeting felt that very few codes would scale to very large processor counts. The ASCI experience USA highlights the fact that it is extremely hard to port legacy code to very high processor counts and that instead codes had to be re-engineered from the start. Unless a large commitment to code development is forthcoming as part of the planned procurement the working group felt that it would rather see Hector being a set of mid-range (512/1024 processor) boxes coupled together. This would not preclude the use of all the clusters for very large calculations but would enable us to exploit the box far more easily than, for example, we could a single 10,000 processor box.

## 7 DLV Status Report

BGS reported in the current status of DLV including the release of v2.4 and the current work preparing for v3.0. BGS was thanked for his work.

## 8 DL\_EXCURV Status Report

ST reported on his current work on DL\_EXCURV which lead to a full release in August 2004. The working group congratulated him on his efforts so far. The key deliverable from this work is the release of self-consistent phase shifts. Initial testing and validation of possible methodologies is currently underway.

Full details of the DL\_EXCURV package are available via  
<http://www.cse.clrc.ac.uk/cmng/EXCURV/>

Since the codes release in August 38 licences have been issued which is an impressive take up of the new code.

## 9 Newsletter

The newsletter was discussed. It was felt that the newsletter was probably out dated and should be discontinued. However, the working group felt that it was important to maintain the flow of information to our user base. This is probably best done electronically.

**Action: AW to install a 'latest news' section on the CCP3 web site**

**Action: AW to initiate a six monthly e-mailing to the registered users containing a short summary of recent news**

## 10 AOB

### 10.1 Student Bursaries

It was suggested that CCP3 should provide student bursares for the forthcoming ISSC meeting in Cardiff and for the ECOSS meeting in Berlin. It was agreed that we would provide three bursaries for each event at the level of 100-00 pounds for ISSC and 150-00 for ECOSS. Preference would be given to those presenting work at the conference.

**Action: ALL - submissions and a short letter of support to AW if you have a student who wishes to apply**

### 10.2 Visitors

A request was received from GPS for three visitors (from Japan, Brazil and Turkey) at a total of 1000-00 for the three. This was agreed.

### **10.3 Date of Next Meeting**

It was suggested that the next meeting could be held in Cardiff during ISSC in June.

**Action: AW to contact JI**

## Action List

1. AW to correct minutes and install on web
2. AJF to continue discussions with PJD regarding DIAMOND
3. NMH, GPS, JI and SC to provide short reports on their visitors to AW asap
4. AJF to discuss possible Russian visitors with LK
5. AJF to invite LK to join the working group
6. NMH and MF to report to the next meeting on the clusters grant
7. AW and RG to investigate excited states and report to the next meeting
8. AJF to contact James Annett to identify a CCP9 organiser for a workshop on magnetic surfaces and liase with WH
9. AJF to liase with John Harding on a possible theme for a joint CCP3/CCP5 workshop
10. AJF to raise the issue of semiconductor physics at next CCP steering panel meeting
11. ALL submit updated lists of visitors/workshops/publications to AW. The current publication list is available via <http://www.ccp3.ac.uk/Coordination/CCP3/pubs.htm>
12. AW to install a 'latest news' section on the CCP3 web site
13. AW to initiate a six monthly e-mailing to the registered users containing a short summary of recent news
14. ALL - submit details and a short letter of support to AW if you have a student who wishes to apply for a student bursary
15. AW to contact JI regarding the venue and date for the next meeting