

# MINUTES OF THE CCP3 WORKING GROUP MEETING

Univeristy College London

Thursday 22<sup>nd</sup> July 2004

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

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## 1 Apologies for absence

Apologies for absence were noted.

## 2 Minutes of the previous meeting (13/09/2003)

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

**Action: AW to install on web**

## 3 Matters Arising

### 3.1 DIAMOND Interactions

AJF has contacted CN about possible CCP3/DIAMOND interactions but has received no reply. It was felt by the meeting that this was an important avenue to explore. It was suggested that AJF should contact Gerhard Materlik and PJD regarding this issue.

**Action: AJF to contact PJD and GM**

### 3.2 Non-linear Optics

In the absence of JI and SC this item was postponed until the next meeting

**Action: JI and SC to report to the next meeting**

### 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**

## 4 Changes to the Working Group

Richard Palmer has stood down from the working group. He was thanked in his absence for his many years of valued service to the CCP.

**Action: AJF to write to RP and thank him for his contributions**

It was agreed that Dr Roy Johnston from Birmingham and Dr Michele Warren from Manchester be invited to join the working group.

**Action: AJF to contact RJ and MW to invite them to participate**

## 5 Grant Updates

### 5.1 Single Molecule Spectroscopy Grant

AJF reported on the status of this grant which is ready for submission. It was agreed that the grant should be submitted as a flagship grant and should include T&S costs for the project from Jan 2006 - Dec 2007. This will be included on the Liverpool section of the grant form.

**Action: AW to liaise with WH regarding wording and costs**

## 5.2 Clusters Grant

In the absence of NMH and MF detailed discussion of this grant was postponed until the next meeting. It was felt that they should liaise with WF, GT, RL and Chris Binns regarding possible experimental tie-ins.

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

## 5.3 Dynamics and Excited States

The proposed workshop has been cancelled as it was felt that the subject matter would be too close to the SRRTNet workshop on FeL's held in May. RG reported on the new European Network on excited states and it was felt that there may be scope for a joint workshop between that network and CCP3.

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

## 5.4 Magnetic Properties of Surfaces

There was a wide ranging discussion concerning the possibility of a new CCP3 project on magnetic surfaces and in particular magnetic semiconductor surfaces. The meeting agreed that a joint theory/experiment workshop on surface magnetism would be helpful and that this could be run as a joint CCP3/CCP9 activity.

**Action: AJF to contact James Annett re CCP3/CCP9 interactions**

**Action: WH to review the experimental and theoretical literature and report to the working group**

## 6 Student Bursaries

A request was received from NMH for Student Bursaries for the forthcoming CRYSTAL training workshop to be held at Imperial College. It was agreed that CCP3 would provide 5 bursaries of up to 150 pounds for this meeting to assist the attendance of UK students at this meeting.

## 7 Visitors

A request was received from NMH for two visitors at the CRYSTAL training workshop at the level of 200 pounds each. The meeting stressed that CCP3 visitors should interact with more than one CCP3 node. NMH was therefore requested to circulate the names of the visitors together with their travel schedules and availability to the working group in order to establish if there will be interactions with other centres.

**Action: NMH to circulate details of speakers**

WH request a visit from Peter Mohn who will be based at Liverpool and will visit York and UCL. The meeting agreed this request at a level of upto 400 pounds.

**Action: WH to invite Peter Mohn and liase with AJF/RG to arrange visits**

AJF requested a visit for a visitor from the Russian centre for non-equilibrium physics. This visit was agreed in principle at a level of up to 400. WH was interested in such a visitor also visiting Liverpool although it was thought that a visit to DL might be more appropriate.

**Action: AJF to circulate details of the visitor and liase with the working group about possible visits to other centres**

## 8 Flagship Grant Report

In ST's absence, AW updated the meeting on the current status of the flagship grant project. The meeting congratulated ST on his progress to date.

## 9 DLV Status Report

BGS presented the current status of DLV to the meeting. This now includes a full interface to DL\_EXCURV.

## 10 CRYSTAL Update

AW presented recent developments in CRYSTAL to the meeting including the release of CRYSTAL2003. A training workshop on CRYSTAL will be held at Imperial College, London during September.

## **11 HECToR Procurement**

The meeting discussed its wish list for the HECToR system. The views of the CCP will be fed back to the procurement panel via AJF

The meeting also discussed a possible CCP3 bid for time on HPCx. There was interest expressed by WH, AJF and PW. GPS has previously also shown interest. This is probably sufficient to consider a small consortium bid for time.

**Action:** AW to contact GPS to confirm interest

## **12 CCP Steering Panel Meeting Report**

AJF reported that Mike Allen had resigned as chairman of the CCP steering panel and that his replacement had not yet been appointed.

## **13 Customer Satisfaction Review**

The recent customer satisfaction report on the CCP's was discussed. The meeting felt that the principle issue CCP3 needed to address was the relatively low take up of the DLV software package.

## **14 Any Other Business**

AW informed the meeting that an SRRTNet workshop on non-UHV Surface Science will be held at DL in November. Several members of the working group suggested possible speakers for the meeting and also expressed an interest in attending.

**Action:** AW to circulate full details once finalised

## **15 Date of Next Meeting**

The meeting will be held on 17/12/2004. Venue to be decided.

## Action List

1. AW to install minutes of the 13/09/03 meeting on the web site
2. AJF to contact Gerhard Materlik and PJD concerning CCP3/DIAMOND interactions
3. JI and SC to report on Non-linear optics to the next working group meeting
4. AJF to thank RP for his services on the working group
5. AJF to contact MW and RJ and invite them to join the working group
6. AW to liase with WH and include working group costs on the spectroscopy grant
7. NMH and MF to report on status of cluster grant at the next meeting
8. AW and RG to report on excited states to the next meeting
9. AJF to contact CCP9 about a possible joint workshop
10. WH to investigate exp and theory literature on surface magnetism and report to the next meeting
11. NMH to circulate details of visitors to the working group
12. WH to invite Peter Mohn to visit and arrange interactions with York/UCL
13. AJF to circulate details of possible Russian visitors
14. AW to contact GPS regarding possible CCP3 HPCx bid
15. AW to circulate details of the SRRTNet workshop when available