

MINUTES OF THE CCP3 WORKING GROUP MEETING

University College London 07/07/2006

Present	Apologies
Prof. A Fisher (Chair)	Prof. D Bird
Dr. A Wander	Dr. P Durham
Dr. BG Searle	Prof. NM Harrison
Dr. W Hofer	Prof. R Godby
Dr S Tomic	Prof. DP Woodruff
Prof. GP Srivastava	Dr EA Colbourn
Prof. C. Norris	Dr. J Blackman
Dr. M Warren	Dr. S Crampin
Prof. G Thornton	Prof. W Flavell
Prof. R. Smith	Prof. J. Inglesfield
Dr. H. Van Damm (CCP1)	Dr. S Holloway
	Dr L Kantorovich
	Dr. R Lambert
	Dr. WC Mackrodt
	Prof. J A D Matthew
	Prof. M. Finnis
	Dr. S Parker
	Dr. S Tear
	Prof. Sir JB Pendry
	Dr. J Purton
	Dr. J Blackman
	Prof P Weightman
	Dr. RL Johnson

1 Apologies for absence

Apologies for absence were noted.

2 Minutes of the previous meeting (17/01/2006)

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

Action: AW to install on web

3 Matters Arising

The F90 course had stalled due to the need to run the course outside of University term time. The working group requested that the course should be run as soon as possible.

Action: AW to arrange dates and venue and contact Peter Coveney for permission to call the course a CCP training event

The workshop on Wet Minerals is progressing. MW and Keith Refson will continue work on this.

Action: MW to report to next working group meeting

4 Changes to the Composition of the Working Group

John Inglesfield has asked to stand down from the working group as he will be retiring shortly. He was warmly thanked for his long service and many contributions to the CCP as a member of the working group and as its chairman.

John Jefferson has been approached and was willing to join the working group although he was not directly involved with surface science.

Action: AW to update web pages and mailing lists

Rob Lindsay of the University of Manchester was proposed as a new member of the working group. Rob is an experimentalist with expertise in LEED and synchrotron radiation studies of surfaces.

**Action: AJF to contact and invite Rob to join
(robert.lindsay@manchester.ac.uk)**

Dr. Sarnjeet Dhesi and Dr. Chris Nicklin from Diamond were proposed as members of the working group. Sarnjeet is developing the nano-science beamline and Chris is working on the Surface and Interface Diffraction beamline.

**Action: AJF to contact and invite Sarnjeet
(sarnjeet.dhesi@diamond.ac.uk) and Chris
(chris.nicklin@diamond.ac.uk) to join the working group**

5 Diamond Interactions

CN detailed the beamline developments of Diamond that overlap with the interests of CCP3. First users of the facility are anticipated in early 2007. Diamond will have approximately 6 staff and 6 PDRA's working in the area of Surface Science. It is important that the working group seeks to identify joint areas of interest in order to enable us to respond to the needs of the user community and of the Diamond scientists in a timely and appropriate manner. This process will be enhanced by the addition of Sarnjeet and Chris to the working group (see previous section).

6 Grant Updates

6.1 HPCx Grant

This grant has been submitted and we await referees comments

6.2 CCP1/CCP3 Grant

Huub Van Dam attended the meeting on behalf of CCP1. There are obvious developmental targets and it seems likely that the CCP steering panel would be supportive of such a joint bid particularly if it makes use of the new CCP source forge types of activities. It is important that the code development is packaged as enabling science and the key scientific targets were seen as photocatalysis and pump probe spectroscopy.

Action: GT to feed in photocatalysis material. AW and HvD to develop case

6.3 LightNeT

The contracts have now been issued and the grant will therefore start shortly.

6.4 DEISA

The DEISA proposal was noted and member of the working group were asked to contact AW asap and if they wished to take a joint bid forward

Action: ALL - contact AW by 10/07/06

Action List

7 Student Bursaries

It was requested that CCP3 should provide bursaries for the ICNT meeting in Basle. This was agreed at the level of 250-00

8 Visitors

Hon Cho (sp?) will visit Liverpool and John Rehr will visit DL. Funding for both visits of up to 500-00 was agreed.

9 DLV Status Report

DLV v3.0 is now in beta release and will be presented at the forthcoming CRYSTAL workshop in Turin (Sept 06).

10 Flagship Grant Report

The flagship grant on single molecule spectroscopy is progressing well.

11 SESP

AW reported on the current status of SESP and asked for a volunteer to try the available tools. RS was keen.

Action: AW to liase with RS and arrange a vist to RAL to try out the available tools

12 AOB

SP forwarded a request for CCP3 to provide support for BM's retirement meeting. This was agreed at a level to be determined.

The next meeting will be held in early/mid January

Action: AW to arrange date and venue

1. AW to install minutes of the previous meeting on the web
2. AW to arrange dates and venue for the F90 course
3. MW to continue work on Wet Minerals workshop and report to next meeting

4. AW to update web pages/ mailing lists to reflect the new composition of the working group
5. AJF to contact Rob Lindsay, Sarnjeet Dhesi and Chris Nicklin and invite them to join
6. AJF to write to JI thanking him for his many contributions to the CCP
7. GT to send AW details of experimental photocatalysis bid
8. AW to liaise with HvD and prepare bid
9. ALL - contact AW by 10/07/06 if interested in DEISA bid
10. AW to liaise with RS and arrange a visit to RAL to try out the available tools
11. AW to arrange date and venue for next meeting