

# Daresbury Laboratory

## INFORMATION NEWSLETTER

### FOR COMPUTER SIMULATION

### OF CONDENSED PHASES

An informal Newsletter associated with Collaborative Computational Project No.5  
on Molecular Dynamics, Monte Carlo & Lattice Simulations of Condensed Phases.

Number 46

October 1998

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Editor: Dr. M. Leslie

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## General News

### **CHAIRMANSHIP OF CCP5 AND MEMBERSHIP OF EXECUTIVE COMMITTEE**

Following a ballot by Email of UK members of CCP5, a new chairman was elected in February of this year. Four new executive committee members have also been elected in September. Professor M. Allen had held the post of chairman for the past two and a half years. The executive committee members who have retired are

- M. Finnis (Atomistic Simulation Group, Queen's University Belfast)
- C. Care (Materials Research Institute, Sheffield Hallam University)
- M. Stapleton (Molecular Simulations)

A table giving contact details for the current executive committee is given on the next page.

Table 1: CCP5 Executive Committee Members

Name Period of Service	Address	Email, Telephone Fax, WWW
Chairman Dr. D.M. Heyes 1996 - 1999	Department of Chemistry University of Surrey Guildford GU2 5XH	d.heyas@surrey.ac.uk +44 (0) 1483 259580 +44 (0) 1483 259514 <a href="http://www.chem.surrey.ac.uk/~chs1dh/">http://www.chem.surrey.ac.uk/~chs1dh/</a>
Secretary Dr. M. Leslie 1983 -	Daresbury Laboratory Daresbury, Warrington Cheshire WA4 4AD	m.leslie@dl.ac.uk +44 (0) 1925 603507 +44 (0) 1925 603634 <a href="http://www.dci.rl.ac.uk/Person.asp?m.leslie">http://www.dci.rl.ac.uk/Person.asp?m.leslie</a>
Dr. W. Smith 1980 -	Daresbury Laboratory Daresbury, Warrington Cheshire WA4 4AD	w.smith@dl.ac.uk +44 (0) 1925 603257 +44 (0) 1925 603634 <a href="http://www.dci.rl.ac.uk/Person.asp?w.smith">http://www.dci.rl.ac.uk/Person.asp?w.smith</a>
Dr. J. Anwar 1998 - 2001	Department of Pharmacy Kings College London London SW3 6LX	jamshed.anwar@kcl.ac.uk +44 (0) 171 333 4782 +44 (0) 171 351 5307 <a href="http://www.kcl.ac.uk/kis/schools/life_sciences/health/pharmacy/staff/anwar.html">http://www.kcl.ac.uk/kis/schools/life_sciences/health/pharmacy/staff/anwar.html</a>
Dr. J. Gale 1998 - 2001	Dept. of Chemistry Imperial College London SW7 2AY	j.gale@ic.ac.uk +44 (0) 171 594 5757 +44 (0) 171 594 5804 <a href="http://www.ch.ic.ac.uk/gale/.index.html">http://www.ch.ic.ac.uk/gale/.index.html</a>
Dr. J.H. Harding 1996 - 1999	Materials Research Centre University College London London WC1E 6BT	j.harding@ucl.ac.uk +44 (0) 171 419 3506 +44 (0) 171 391 1360 <a href="http://www.phys.ucl.ac.uk/~cmmmp/">http://www.phys.ucl.ac.uk/~cmmmp/</a>
Dr. J. Melrose 1998 - 2001	Polymer and Colloid Group, Cavendish Lab University of Cambridge Cambridge CB3 0HE	jrm23@phy.cam.ac.uk +44 (0) 1223 337263 +44 (0) 1223 337000 <a href="http://www.poco.phy.cam.ac.uk/~jrm23/">http://www.poco.phy.cam.ac.uk/~jrm23/</a>
Prof. G.S. Pawley 1996 - 1999	Department of Physics University of Edinburgh Edinburgh EH9 3JZ	g.s.pawley@edinburgh.ac.uk +44 (0) 131 650 5300 +44 (0) 131 650 5212 <a href="http://www.ph.ed.ac.uk/cmatter">http://www.ph.ed.ac.uk/cmatter</a>
Prof. A.P. Sutton 1998 - 2001	Department of Materials University of Oxford Oxford OX1 3PH	adrian.sutton@materials.ox.ac.uk +44 (0) 1865 273770 +44 (0) 1865 273783 <a href="http://units.ox.ac.uk/departments/materials/MML/People/Sutton.html">http://units.ox.ac.uk/departments/materials/MML/People/Sutton.html</a>

## FUTURE MEETINGS

A summary table is given below, further details may be found on the WWW pages.

TOPIC	DATES	LOCATION	ORGANISER
URL			
Physical Chemistry in the Mesoscopic Regime	12-14 April 1999	Chester, UK	Royal Society of Chemistry
<a href="http://chemistry.rsc.org/is/journals/current/faraday/fadmeet.htm">http://chemistry.rsc.org/is/journals/current/faraday/fadmeet.htm</a>			
World Association of Theoretically Oriented Chemists	1-6 August 1999	London	WATOC
<a href="http://www.chemsoc.org/watoc99/">http://www.chemsoc.org/watoc99/</a>			
Surface Science of Metal Oxides	1-3 September 1999	Ambleside, UK	Royal Society of Chemistry
<a href="http://chemistry.rsc.org/is/journals/current/faraday/fadmeet.htm">http://chemistry.rsc.org/is/journals/current/faraday/fadmeet.htm</a>			

## CCP5 FUNDS FOR COLLABORATIONS

CCP5 can make available funds of up to £200 per annum for groups of two or more UK researchers wishing to undertake a collaborative project within the scientific area covered by CCP5. The funds are intended to cover travel and subsistence costs. Researchers who wish to apply for funds are requested to submit a brief proposal (about 1/2 a page) describing the intended work to Dr. M. Leslie at the address below.

## CCP5 VISITORS PROGRAM

CCP5 organizes a visitors program which funds the visit to the UK of overseas collaborators. We would normally expect a visitor to visit three sites in the UK and give a lecture at each site. These lectures would be open to all members of CCP5 as well as members of the host university. The visit would normally last between one or two weeks. CCP5 would pay for the cost of travel to the UK and within the UK between universities. CCP5 would expect some contribution towards accommodation expenses at the host university to be met by the university. We will also consider longer collaborations or visits just one place if this can be justified by the nature of the work to be done. If you have an overseas collaborator who you would like to invite under this program, please make a request to Dr. M. Leslie.

## ELECTRONIC DISTRIBUTION OF CCP5 NEWSLETTERS AND WORLD WIDE WEB

All newsletters starting from issue 39 (October 1993) are now available on line, together with some articles from earlier newsletters. An index of recent newsletter articles can be found on the World Wide Web server; readers can access the individual articles by this means or by anonymous ftp. (Anonymous ftp will not access the index). The URL for the CCP5 home page is <http://www.dl.ac.uk/CCP/CCP5/main.html>

### HOW TO GET THIS NEWSLETTER BY FTP

- |    |                                                |                                 |
|----|------------------------------------------------|---------------------------------|
| 1. | move to the desired directory on YOUR machine  |                                 |
| 2. | type:                                          | ftp ftp.dl.ac.uk                |
|    | or                                             | ftp 148.79.80.10                |
| 3. | enter userid:                                  | anonymous                       |
| 4. | enter passwd:                                  | <i>enter your name and site</i> |
| 5. | change to ccp5.newsletters/46 directory:       | cd ccp5.newsletters/46          |
| 6. | change to postscript or latex subdirectory     | cd ps                           |
|    | or                                             | cd latex                        |
| 7. | to get the required files from the directory : |                                 |
|    | postscript from ps directory                   | get nl.ps                       |
|    | compressed postscript from ps directory        | get nl.ps.gz                    |
|    | latex from latex directory                     | get nl.tex                      |
| 8. |                                                | quit                            |

Below is an index of the information held.

Readers may now **register** by filling in an on-line WWW form. Existing readers may also notify registration changes in this way.

In addition to notification of newsletters, we occasionally send other messages about meetings to the Email list. If you want us to send **notification of newsletters only**, let me know and I will place your Email address on a separate list. This will allow readers to restrict the amount of incoming Email if this will be a problem due to limited bandwidth or if readers are charged for incoming Email.

This newsletter is available by anonymous ftp either directly or by accessing the Daresbury World Wide Web server. The newsletter has been placed (in separate directories) both as postscript files and as the source latex files.

## INFORMATION ON WWW SERVER

History of the project.

Organisation of the project.

Current research interests .

A library of computer software maintained by the project.

An index of future meetings and workshops which CCP5 is involved in organising or has been asked to publicize.

A list of proposed visitors sponsored by CCP5 with itinerary.

An index of articles from recent issues of the newsletter.

A copy of recently published newsletters commencing with Issue 39 (October 1993).

Registration and de-registration details.

Other related information on the Web.

## Distribution of Information by Email

CCP5 will distribute by Email to the members on the mailing list (about 850 world wide) information which is of interest to our members. Three lists are maintained, for UK members, members in other European countries and all other members. If you have information which you would like sent out in this way please send it by Email to M. Leslie, indicating whether it would be appropriate to restrict its distribution. We also send out post-graduate, post-doctorate and lectureship positions notified to us. Normally the Email messages for post-graduate positions within the UK are restricted to UK members, however if the position is open to non-UK students then Email may be sent to the rest of Europe or the complete mailing list. Messages sent out may be batched together in which case there may be a short delay between the receipt of the message at Daresbury and its transmission. CCP5 no longer places the positions on the WWW or ftp servers but a link will be placed from CCP5's page to a page at a University advertising the position.

## THE CCP5 PROGRAM LIBRARY

Copies of the newsletter no longer include a complete description of the program library. If readers wish to obtain a copy of the documentation it is available by anonymous ftp or through the World Wide Web page. The program library description is in `ccp5.newsletters/library` directory (postscript and ASCII text versions).

## REQUEST FOR CONTRIBUTIONS

Contributors to the current issue

Our thanks go to:

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The deadline for contributions for the next newsletter will be **1 April 1999**. Readers are reminded that contributions are always welcome. Contributions may be sent by Email in  $\text{L}^{\text{A}}\text{T}_{\text{E}}\text{X}$ . WORD documents should preferably be sent in rtf format.

### Address

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