

# Daresbury Laboratory

# INFORMATION QUARTERLY 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 44

July 1995

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## Contents

• General News	3
• Meeting and workshop announcements	9
• Structure and Order in Liquids	9
• Simulation of molecular materials	10
• Advanced Computer Simulation of Materials	11
• Recent Advances in Molecular Simulation	15
• Job Vacancies	16
• The CCP5 Spring school	18
M. P. Allen	

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Editor: Dr. M. Leslie

CCL Daresbury Laboratory  
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## Contents (continued)

- Modelling of Localised States in Condensed Matter 20  
L. Kantorovich
- Singularity-free Treatment of Linear Bond Angles 40  
F. Müller-Plathe
- A Novel Application for Molecular Dynamics - The Simulation of Powder Flow 42  
D.M. Heyes, P.A. Langston and U. Tüzün
- Car-Parrinello Simulation Reveals Complex Ions in Liquid Semiconductors 53  
M. J. Gillan, F. Kirchhoff and J. M. Holender

## General News

### CHAIRMANSHIP OF CCP5

Following a ballot by Email of UK members of CCP5, a new chairman and three new executive committee members have been elected. Professor M. Gillan has held the post of chairman for the past two and a half years. The executive committee members who have retired are

M. Allen (Physics, Bristol)  
J. Goodfellow (Crystallography, Birkbeck)  
W. Mackrodt (Chemistry, St. Andrews)

and the three members who will continue to serve are

G. Jackson (Chemistry, Sheffield)  
G. D. Price (Geology, UCL)  
S. Parker (Chemistry, Bath)

The result of the ballot is given below

CHAIRMAN		
Person nominated	Institution	Votes
M. Allen	Department of Physics, Bristol	23 (Elected)
J. Harding	AEA Technology, Harwell	5
N. Quirke	University of Bangor	13

EXECUTIVE COMMITTEE		
Person nominated	Institution	Votes
C. Care	Materials research Institute, Sheffield Hallam	21 (Elected)
M. Finnis	Queen's University, Belfast	25 (Elected)
J. Gale	Imperial College, London	15
R. Grimes	Department of Materials, Imperial College, London	13
J. Harding	AEA Technology, Harwell	19
M. Stapleton	MSI, Cambridge	23 (Elected)

### FUTURE MEETINGS

A summary table is given below, further details may be found inside.

TOPIC	DATES	LOCATION	ORGANISER
Structure and Order in Liquids	22-27 September 1995	Blankenberge	European Science Foundation / European Molecular Liquids group
Simulation of Molecular Materials	6 September 1995	Sheffield	Royal Society of Chemistry
Advanced Computer Simulation of Materials	20-22 September 1995	Daresbury	CCP5
Recent Advances in Molecular Simulation	6 December 1995	London	Royal Society of Chemistry

Full details of the ESF conference program may be obtained from  
 Dr. Josip Hendekovic, Email euresco@esf.c-strasbourg.fr  
 European Science Foundation,  
 1 quai Lezay-Marnésia, Tel. +33 88 76 71 35  
 67080 Strasbourg Cedex, Fax +33 88 36 69 87  
 France

## CRAY NEWS

CCP5 participants are reminded that CCP5 has an annual allocation of Cray time at Rutherford Laboratory. This is available for the development of simulation programs which are of general use to the CCP5 community. Readers who wish to use some of this allocation should write to the CCP5 Secretary, Dr. M. Leslie.

## INTEL NEWS

CCP5 also has an annual allocation of time on the Intel IPSC/860 at Daresbury. If any CCP5 member wishes to make use of some of this time please contact M. Leslie at Daresbury.

## 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/44 directory:       | cd ccp5.newsletters/44          |
| 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.

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.

Job vacancies

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

The section on other related information has been expanded, and I will add any further links notified to me.

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.

## **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).

## REORGANISATION OF SCIENCE IN THE UK

Following reorganisation, Daresbury Laboratory is now part of “The Central Laboratory of the Research Councils”, together with Rutherford Appleton Laboratory in Oxfordshire. The postal address is given below.

## REQUEST FOR CONTRIBUTIONS

Contributors to the current issue

Our thanks go to:

Dr. M. Allen	Department of Physics University of Bristol
L. Kantorovich	Physics Department Keele University Keele, Staffordshire ST5 5BG, U.K.
F. Müller-Plathe	Laboratorium für Physikalische Chemie ETH-Zentrum Zürich Switzerland
D.M. Heyes P.A. Langston U. Tüzün	Department of Chemistry University of Surrey Guildford GU2 5XH, UK
M. J. Gillan F. Kirchoff J. M. Holender	Physics Department Keele University Keele, Staffordshire ST5 5BG, U.K.

The deadline for contributions for the next 2 newsletters will be **1 September 1995 and 1 December 1995**. Readers are reminded that contributions are always welcome. Contributions may be sent by Email in  $\text{\LaTeX}$ . WORD documents should preferably be sent in rtf format. We would be prepared to consider other formats on a trial basis.

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## MEETING AND WORKSHOP ANNOUNCEMENTS

### RESEARCH CONFERENCE ON

#### MOLECULAR LIQUIDS:

#### Structure and Order in Liquids

A European Research Conference run by the European Science Foundation in association with the European Molecular Liquids Group.

Blankenberge, Belgium, 22-27 September 1995

**Chairman:** R.M.Lynden-Bell (Cambridge)  
**Vice-Chairman:** G.Palinkas (Budapest)

This meeting is the second Euroconference on Molecular Liquids held in association with the European Molecular Liquids Group. Although liquids are disordered on the large scale there is considerable order at the molecular scale. At this meeting there will be discussion of recent experimental and simulation results on local order in liquids and solutions. Both freezing into an ordered crystalline phase and glass formation are affected by the degree of local order and there will be sessions on these topics. The aim of the meeting will be to give a clear picture of the current state of theory and experiment and to highlight areas of future research. Participants are encouraged to contribute to the discussion and poster sessions.

#### Preliminary Programme

##### Order in Liquids

D.Frenkel	(Amsterdam):	Local order and molecular shape.
I.Cabaço	(Lisboa):	Neutron studies of benzene and perfluorobenzene.
MA.Ricci	(Roma):	The structure of water above its boiling point.
H.Versmold	(Aachen):	Investigation of local structure in fluids by light scattering.

##### Solvation

ADJ Haymet	(Sydney):	Calculating the dissociation of water.
E. Guardia	(Barcelona):	Computer Simulation of Ions in Solution.
H.Wengärtner	(Karlsruhe):	Liquid-liquid phase separation and criticality in electrolytes.
P.M.Rodger	(Reading):	Solvent induced structure of the solvation shell.

### Freezing and Melting

- D.Oxtoby (Chicago): Density functional theory of crystallization dynamics.  
P.Madden (Oxford): Nucleation in hard sphere liquids.  
C.Körber (München): Freezing of aqueous solutions - the advancing solid-liquid interface.  
J-P. Hansen (Lyon): Studies of a sol-gel system.

### Glass formation

- L.Sjögren (Göteborg): Mode Coupling theory of glass formation.  
D.Kivelson (Los Angeles): Supercooled liquids and glasses: A thermodynamic theory?  
R.Vallauri (Firenze): Dynamics of supercooled liquids and glasses through normal modes.

## SIMULATION OF MOLECULAR MATERIALS

Royal Society of Chemistry Autumn Meeting,  
Sheffield,  
6 September 1995.

Invited Speakers are:

- Julian Clarke ( Manchester )  
Alejandro Gil ( Sheffield )  
Mike Klein ( Pennsylvania )  
Neal Skipper ( University College, London )  
Dominic Tildesley ( Southampton )

There is space for short contributions.

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Sheffield S3 7HF           E-Mail:   G.Jackson@sheffield.ac.uk  
United Kingdom

## **ADVANCED COMPUTER SIMULATION OF MATERIALS**

**The CCP5 Annual Meeting  
20th - 22nd September 1995  
Daresbury Laboratory, U.K.**

The 1995 Annual Meeting of CCP5 has the theme of 'Advanced Computer Simulation of Materials'. Recent advances in computer power, particularly using parallel architectures, are enormously expanding the range of scientific problems that can be addressed by atomic-scale simulation. The meeting aims to review current research and to explore future possibilities. Ab initio and other quantum-based simulation methods as well as more traditional classical simulation techniques will fall within the scope of the meeting. There will be an emphasis on materials problems, but - as with all CCP5 Annual Meetings - general contributions will be welcome.

### **Invited speakers**

The following speakers are confirmed. Details of the other invited speakers and titles of talks will be forwarded as they become available.

Dr. R. Jones,	Exeter University	The Importance of Combined Modelling and Experimental Studies for Characterising Semiconductors
Prof. U. Landman	Georgia Institute of Technology	To follow
Prof. R. Nieminen	Helsinki University of Technology	Defects, Interfaces and Metastability in Compound Semiconductors
Prof. D. G. Pettifor	Oxford University	To follow
Prof. K. Schwarz	Technical University Vienna	Molecular dynamics simulations of methanol in zeolites

## Organising Committee

M. J. Gillan

G. D. Price

M. Leslie

P. J. D. Lindan

Further information may be found on WWW at  
<http://www.dl.ac.uk/CCP/CCP5/meetings/1995.html>  
or by contacting:

Dr. M. Leslie

Email

m.leslie@dl.ac.uk

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The meeting will start at 14.00 on Wednesday 20 September and finish at 16.00 on Friday 22 September. The closing date for registration and receipt of contributed papers is 31 August 1995.

# REGISTRATION FORM

Advanced Computer Simulation of Materials

Daresbury Laboratory, UK

September 20th. - September 22nd 1995

SURNAME: (Prof , Dr , Mr , Mrs , Miss , Ms \*) ..... Male/Female\*  
(BLOCK letters please). \* Please delete INITIALS: .....

ADDRESS: .....  
.....  
.....  
.....  
.....

Tel ..... Fax .....

Electronic Mail Address .....

Accommodation will be on site at Daresbury Laboratory. The price below for accommodation will be limited to the first 50 delegates only in the order that registration and payment is received. Additional delegates will need to be accommodated in local hotels and will have to pay a supplement which will be about 15.00 pounds per night. Delegates wishing to stay on the night of September 19th. may also need to be accommodated in a local hotel. The accommodation fee includes the price of breakfast on the 21st. and 22nd. of September. Both hot and cold lunches may be purchased on all three days in the laboratory restaurant. Dinner on the 20th. and, for those not attending the Conference Dinner, on the 21st., may also be purchased at the restaurant.

Please indicate if you have any special requirements (Diet, disability)

.....

## CONFERENCE COSTS

(Prices in Pounds Stirling)

- 1) Conference Fees (please circle as appropriate) (Graduate students will need to send a supporting letter from the supervisor to qualify for the discount)

Non-Student	£40	.....
Graduate Student	£0	.....

- 2) Accommodation on night of Wednesday September 20th. (Bed and Break- £23.00 .....  
fast only)
- 3) Accommodation on night of Thursday September 21st. (Bed and Break- £23.00 .....  
fast only)
- 4) I will require additional nights accommodation on (please circle as  
appropriate)  
September 19th.  
September 22nd.  
(Payment for additional nights may be made at the conference)
- 5) Conference Dinner on Thursday 21st. September £15.00 .....

I enclose a cheque for total £ ..... (Payable to “Daresbury Laboratory”).

### CONFERENCE PRESENTATIONS

I would like to submit a presentation Yes/No\*

I would prefer an ORAL/POSTER\* presentation

Oral presentations will be 30 minutes including time for questions. Posters will be presented on display boards measuring 90cm x 115 cm.

TITLE .....

Lead author: .....

Affiliation: .....

Co-author(s): .....

Affiliation(s): .....

An abstract must be sent at the time of registration by electronic mail in an electronic format. The preferred formats are either LATEX or WORD. (If you use WORD, please send the file in RTF format). We may be able to accept other word processor formats; please contact the organisers. The abstracts will be published as part of an issue of the CCP5 quarterly newsletter. Delegates are also encouraged to submit a longer account of their work for publication in the newsletter. Postscript diagrams may also be accepted.

### TRAVEL ARRANGEMENTS

I will arrive by car Yes/No\* Registration number .....

Please send a map Yes/No\*

If you are travelling by rail, the closest stations are Runcorn and Warrington Bank Quay on the main line from London, Euston. By air, Manchester airport is 15 miles away from the laboratory. Please return by 31 August to Dr. M. Leslie, CCL Daresbury Laboratory, Warrington, WA4 4AD, UK.

Royal Society of Chemistry: Theoretical Chemistry Group  
Statistical Mechanics and Thermodynamics Group and  
EPSRC Collaborative Computational Project No. 5:  
Computer Simulation of Condensed Phases

## THEORETICAL CHEMISTRY DAYS No. 3: RECENT ADVANCES IN MOLECULAR SIMULATION

A half-Day meeting to be held in the Department of Chemistry, University College, London on Wednesday 6th December 1995, from 13.30 to 17.10.

### Programme

1330	Chairman's Introduction	Professor J. N. L. Connor	(University of Manchester)
1340	Keynote Lecture: Molecular Simulation: Recent Advances.	Professor D. J. Tildesley	(University of Southampton).
1430	Simulation of Polymers: Recent Advances.	Professor J. H. R. Clarke	(UMIST).
1455	Tea		
1530	Plenary Lecture: Molecular Dynamics from First Principles: Recent Advances.	Professor R. Car	(Ecole Polytechnique Federale de Lausanne, Switzerland).
1620	Simulation of Stretched Crystals: Recent Advances	Professor R. M. Lynden-Bell	(Queen's University, Belfast).
1645	Simulation of Liquid Crystals: Recent Advances	Doctor M. P. Allen	(University of Bristol).
1710	Close		

Organiser:

Professor J. N. L. Connor, Department of Chemistry, University of Manchester, Manchester M13 9PL.

Local Organiser:

Doctor Sally Price, University College London.

**Post Doctoral Position**  
**Oxford University Department of Earth Sciences**  
**Postdoc in ab-initio Simulations of Alumino-Silicates**

We are seeking to fill a position for a postdoctoral research assistant to work on Earth materials science problems involving alumino-silicate and oxide minerals. The work will use total energy pseudopotential methods and will form part of a program of study of order/disorder and water/mineral interaction processes, though there will be some flexibility regarding the specific problems to be tackled. The Earth Sciences department has substantial local computing equipment, although some parts of the work may require the use of national supercomputing facilities.

The exact duration will depend on which salary point the appointment is made at and therefore on the age and experience of the candidate, but will be approximately 16 months. The post will begin at a date in the near future by arrangement.

Candidates must have a sound theoretical background and a PhD in a relevant discipline. Experience with electronic structure calculations will be an advantage. To apply, please send your CV and letter of application to

Professor J. D. C. McConnell  
Department of Earth Sciences  
Parks Road  
Oxford OX1 3PR

or by email (PostScript or LaTeX are acceptable but PLEASE make sure the document is portable!) to me, "Keith.Refson@earth.ox.ac.uk".

**Daresbury Laboratory**  
**Modelling of the Physical Properties and Catalytic Activity of Zeolite**  
**Materials**

Applications are invited for a two-year fixed-term position within the Theory and Computational Science (TCS) Division at the CCL Daresbury Laboratory, Warrington, UK.

TCS Division works closely with experimentalists using the Synchrotron Radiation Source, with theoretical groups in Universities, and with industry. The Division is a recognised leader in the scientific exploitation of high performance computing; strong emphasis is placed on the development of effective parallelised scientific applications codes.

The position, which is part of a collaboration with Unilever Port Sunlight Laboratory, will involve the development and application of techniques for the modelling of the physical properties and catalytic activity of zeolite materials. Classical simulation, solid-state and molecular quantum-mechanical (HF, DFT) techniques will be used, with emphasis on models that link a quantum

mechanical treatment of the active site with a classical molecular mechanical (MM) treatment of region of the surrounding zeolite lattice. With such models, it is possible to treat the active site with high-level quantum chemical methods, which are capable of dealing with the breaking of chemical bonds, while the long-range electrostatic effects of the zeolite framework and the flexibility of the lattice are accounted for using much cheaper classical approximations.

The appointee to the position will be expected to contribute both to the development of the methods required and in the application of these methods to problems of interest. The development aspect of the work will require the modification of existing codes and the writing of new code modules as required, together with the design of test problems to validate and calibrate the new methods. The applications work will involve both the re-examination of problems from the experimental and computational literature using new methodologies, as well as work in close collaboration with Unilever on problems of more direct commercial relevance.

The successful candidates will be expected to have a PhD in a relevant area of computational science, with preference will be given to those candidates with experience in quantum chemistry of molecules and/or solid-state materials.

The salary will be in the range 13 025 - 18 911 pounds sterling depending on qualifications and experience. The laboratory operates a no smoking policy.

Further information may be obtained from Dr P. Sherwood (phone +44 (0)1925 603553, FAX +44 (0)1925 603634, email p.sherwood @dl.ac.uk), Dr N. M. Harrison (+44 (0)1925 603334 n.m.harrison @dl.ac.uk) or, at Unilever, Dr Steve Loades (s\_loades @urpsl.co.uk, +44 (0)151 471 3191)

Application forms may be obtained from:

The Personnel Officer,  
Daresbury Laboratory,  
Warrington,  
Cheshire, WA4 4AD.  
Phone +44 (0)1925 603467 (24 hour answering service)

quoting reference DL321. The closing date for applications is Friday 11th August, 1995.

Daresbury Laboratory is part of the Council for the Central Laboratory of the Research Councils.