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 43 February 1995

Contents

Editor: Dr. M. Leslie

DRAL Daresbury Laboratory
Daresbury, Warrington WA4 4AD UK

Contents (continued)

General News

Hardware failure

Due to a hardware failure, anonymous ftp and WWW access to the program library and newsletters was not available for an extended period during late December 1994. Please accept our apologies for any difficulties this may have caused.

UK Telephone numbers

All telephone numbers in the UK have changed; however the existing numbers will continue to work until April 1995. To make the change, insert an extra digit 1 after the international code (44) but before the local area code. The Daresbury telephone number is noted in full below.

FUTURE MEETINGS

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

TOPIC	DATES	LOCATION	ORGANISER
The Structure and Properties of Oxide Surfaces	5-6 April 1995	Daresbury	CCP3
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

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

Below is an index of the information held.

History of the project.

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:	*enter your name and site*
5.	change to ccp5.newsletters/43 directory:	cd ccp5.newsletters/43
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

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).

Users of fast Fourier transforms may like to note the following. Keith Refson from the Earth Sciences Department, Oxford, has been carrying out timing tests on a FORTRAN implementation of Clive Temperton's GPFA FFT algorithms (C. Temperton, Siam J. Sci. Stat. Comput 13(3), 676-686 (1992)) and has found very favourable performance compared with existing Fortran implementations.

REQUEST FOR CONTRIBUTIONS

Contributors to the current issue

Our thanks go to:

Ramzi Kutteh	Pacific Northwest Laboratory, Richland, WA 99352 USA
P. Lindan N. Harrison W. Smith T. Forester	DRAL Daresbury Laboratory Warrington WA4 4AD UK

Dr. D. Gay	The Royal Institution,
Dr. A. Rohl	London
Dr. M. Allen	Department of Physics
M. Warren	University of Bristol
Dr. M. Wilson	Lancaster University
Dr. A. Sauron	Sheffield Hallam University
Dr. K. Gubbins	Cornell University

The deadline for contributions for the next 2 newsletters will be **1 May 1995 and 1 August 1995** Readers are reminded that contributions are always welcome. This newsletter was delayed because the editor had insufficient material. Contributions may be sent by Email in LaTeX . WORD documents should preferably be sent in rtf format. We would be prepared to consider other formats on a trial basis.

Address

Dr. M. Leslie	Email	
DRAL Daresbury Laboratory,	INTERNET:	m.leslie@dl.ac.uk
Daresbury	BITNET:	m.leslie%dl.ac.uk@ukacrl
Warrington	Tel. +44 (0) 1925 603334	
WA4 4AD	Fax +44 (0) 1925 603634	
UK		

MEETING AND WORKSHOP ANNOUNCEMENTS

THE STRUCTURE AND PROPERTIES OF OXIDE SURFACES

Daresbury Laboratory April 5-6, 1995

This workshop is being organised by CCP3, but is in the area of interest of CCP5. This informal workshop is concerned with recent progress in the theoretical and experimental description of oxide surfaces and interfaces. The topics which will be covered include:

- Recent progress in the first principles description of surface structure and spectroscopy
- Simulation of complex processes at surfaces; molecular adsorption and diffusion.
- Advances in experimental techniques; diffraction and real space imaging.
- The applicability of empirical models.

A registration form, schedule, and some general information are attached below.
Postscript versions of these forms are available on request or by;

1. anonymous ftp to "ftp.dl.ac.uk/ccp3"
2. The WWW page "http://www.dl.ac.uk/CCP/CCP3/main.html"

The registration fees can be paid at the registration desk or by (sterling) cheque payable to "Daresbury Laboratory".

Deadlines: The form must be returned (by post or EMAIL) by 13th March.

Schedule

Wednesday 5th April 1995

10	COFFEE		
10-30	Opening Remarks	N.Harrison	(Daresbury)
11	Exploring oxide surfaces with density functional theory	M Gillan	(Keele)
12	A comparison of different models in the study of chemisorption in infinite systems.	R.Dovesi	(Torino)
1 - 2	LUNCH		
2	Calculation of properties of an oxide/metal interface	M Finnis	(Stuttgart)
3	Ab initio, classical and analytic approaches to oxide surface structure	N Harrison	(Daresbury)

4	COFFEE		
4-30	Contributed talk The calculation of STM images as a tool for interpreting STM data and for understanding geochemical surface reactions at an atomic level.	U Becker	(Virginia)
5.00	Contributed talk.		
5.30	Poster session		
7.00	Discussion / Refreshments		
8.00	Conference Dinner		
	Thursday 6th April 1995:		
08.30	Simulation studies of the stability of oxide surfaces.	P. Lindan	(Daresbury)
09.30	Classical and quantum calculations of oxide surfaces	W Mackrodt	(St-Andrews)
10.30	COFFEE		
11	Oxygen vacancies on MgO (100) : electronic structure and reconstructions	C Noguera and E. Castanier	(Paris)
12	Contributed talk Modelling the surface structures of silicates and barium sulphates.	D. Gay and AL. Rohl	(Royal Institution)
12.30	Contributed talk Atomistic simulation of atomic force imaging of ionic systems	A. Shluger	(Royal Institution)
1-2	LUNCH		
2	Structure/property relations for TiO_2 surfaces	G Thornton	(Liverpool)
3	The surface structure of MgO revisited	K Refson	(Oxford)
4	General Discussion / Posters		
5	Farewell and Coffee.		

General Information

Attendance and Financial Arrangements

If you wish to attend, please complete and return the enclosed application form as soon as possible and no later than Monday 13 March 1995.

FEE:

The conference fee is 70 pounds for academics and 100 pounds for industrial participants. Lunches and refreshments will be provided, as will a Conference dinner which will be held on Wednesday 5 April at the Laboratory. Please indicate on the attached form if you wish to attend the dinner. Cheques (remitted in pounds sterling) should be made payable to "Daresbury Laboratory".

Accommodation

Accommodation is at the Lord Daresbury Hotel at a cost of 69.00 per night including VAT. Accommodation is available for the nights of Tuesday 4 April and Wednesday 5 April. Further nights may be available on request. Any changes to accommodation must be made well in advance of the meeting by post, fax or e-mail.

Travel

Participants must find their own funds for travel.

Bursaries

A limited number of bursaries are available. Please contact Dr N M Harrison at the postal address below or e-mail n.m.harrison@dl.ac.uk

Office Facilities

There will be an information desk at the meeting where participants will be able to make transport arrangements. There will be NO banking or currency exchange facilities. Postal arrangements will be limited to a mail delivery and pick-up service. There will be a restricted photocopying facility.

Postal address: c/o	DRAL Daresbury Laboratory, Warrington WA4 4AD, England
Telephone:	Warrington (01925) 603235
Fax:	01925 603195

For further information please contact

Dr NM Harrison
Daresbury Laboratory
Daresbury
Warrington
WA4 4AD
United Kingdom
Email: n.harrison@dl.ac.uk, FAX - 44 - (0)1925 603634

Registration Form

DRAL

Daresbury Laboratory

CCP3 MEETING ON OXIDE SURFACES

5 - 6 April 1995

APPLICATION FORM

SURNAME: (Prof , Dr , Mr , Mrs , Ms *) ..... Male/Female*
(BLOCK letters please)
FIRST NAME(S) .....

MAILING ADDRESS of Home Institute or Place of Work: .....

.....

.....

.....

.....

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

Electronic Mail Address .....

D L Staff please state division .....

1. ACCOMMODATION: Please note delegates should settle their bill directly with the Hotel.

1.1. I will require accommodation as follows:
The Lord Daresbury Hotel
Single accommodation: £69.00 including VAT (B & B) Tue 4 April YES/NO*
Single accommodation: £69.00 including VAT (B & B) Wed 5 April YES/NO*
If any further accommodation is required please specify:

1.2. Other Hotels: If all our accommodation has been allocated would you like a list of local hotels where you could make your own arrangements? YES/NO*

2. SPECIAL REQUIREMENTS: Please specify any special requirements such as diet, disability etc.....

3. POSTER SESSION

I/we wish to present a poster YES/NO*
Note: No poster bookings will be accepted without full information below.
Lead Author: .....

Affiliation: .....

Co-Author(s): .....

Affiliation(s): .....

Title: .....

.....

.....

To avoid duplicated poster bookings, has one of your co-authors already applied to exhibit this poster? YES/NO*

4. TRAVEL ARRANGEMENTS

Car: I will arrive by car: YES/NO* My registration No. is
Please send a map: YES/NO* .....

Please return this form to arrive no later than 13 March at:

SAS Conference Office
DRAL Daresbury Laboratory
Warrington WA4 4AD
or e-mail conference@dl.ac.uk
* Please delete where inapplicable

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 though 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.

George JACKSON	Tel:	(0114) 282 4781
Department of Chemistry	Fax:	(0114) 273 8673
University of Sheffield		(0114) 275 0182
Sheffield S3 7HF	E-Mail:	G.Jackson@sheffield.ac.uk
United Kingdom		

Post Doctoral Position

Static and Dynamic Properties of Water

Florence, Italy

A post-doc position is available under a contract with EEC for the study of static and dynamical properties of water. This is for one year to be spent in Florence for doing computer simulation on model systems. Another part of the project includes neutron scattering measurements mainly performed at RAL (supervision Alan Soper and Javier Bermejo). Salary will be in accordance with experience. For further information please contact

R. Vallauri
Istituto di Elettronica Quantistica
(C.N.R)
via Panciatichi 56/30
I-50127 Firenze (Italy)

Tel. ++39/55/416128
Fax ++39/55/414612
E-mail simulieq @ vm.idg.fi.cnr.it

Post Doctoral Position

Molecular Simulation of Zeolites

Paris, France

A postdoctoral position is available at the European Centre for Computational Science and Technology in Paris to study adsorption in zeolites. The research will involve the application of novel molecular simulation methods (grand canonical Monte Carlo and grand canonical molecular dynamics of molecules in zeolite frameworks) to gas adsorption. Close contact will be maintained with related work at the Daresbury Laboratory employing ab initio methods and with scientists at Unilever Research. The position (which will be based in Paris) is available now for one year initially.

Please send email/fax/letters of application/CV to

Prof. Nick QUIRKE
Deputy Director
European Centre for Computational Science and Technology
BIOSYM Technologies Sarl
Parc Club Orsay Universit'e — Tel : 33-1-69 41 99 08
20 rue Jean Rostand — Fax : 33-1-69 41 99 09
91893 Orsay Cedex, France — email nick@biosym.fr

The European Centre

The European Centre for Computational Science and Technology is Biosym's European research centre. It is located in new accommodation in Orsay (south of Paris) adjoining the university campus, in the midst of one of the largest concentrations of academic and government research facilities in the world. The centre has very strong links with local and international research groups including the CEA in Saclay, the Université de Paris, the Institut Français du Pétrole as well as groups in other European countries. Our staff hold professorial positions at major European and North American universities.

The centre has excellent computing facilities including powerful workstations It has the full range of BIOSYM modelling software in both release and prerelease forms as well as state of the art in-house research codes not available elsewhere. As well as a general expertise in modelling software and applications methodologies the centre has special expertise in the adsorption, transport and characterisation of porous media (zeolites, carbons,..), organic films and interfaces; oil field chemistry, catalysis and materials science as well as the prediction of phase equilibria.