

# 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 45

May 1996

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Editor: Dr. M. Leslie

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## General News

### FUTURE MEETINGS

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

| TOPIC   | LOCATION                         | DATES                    | ORGANISER   |
|---|----------------------------------|--------------------------|---|
| CCP5 Annual Meeting<br>CONDENSED MATTER<br>SIMULATION:<br>REALIZING THE<br>POTENTIAL OF THE<br>COMPUTER | Bristol                          | 23-25 September 1996     | CCP5  |
| The 3rd International<br>Conference on Computer<br>Simulation of Radiation<br>Effects in Solids         | Surrey                           | 22-26 July 1996          | COSIRES'96  |
| 2nd European Cray MPP<br>workshop   | Edinburgh                        | 25-26 July 1996          | EPCC  |
| Physics Computing '96   | Krakow                           | 17-21 September 1996     | CYFRONET, Krakow and<br>European Physical Society   |
| Optical, electric and<br>magnetic properties of<br>molecules.   | Cambridge                        | 10-13 July 1997          |   |
| Solid State Chemistry: New<br>Opportunities from<br>Computer Simulations                                | University<br>College,<br>London | 30 June - 2<br>July 1997 | The Royal Society of<br>Chemistry, Faraday Division |

### INTEL NEWS

CCP5 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.

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.

### **Distribution of Information by Email**

CCP5 will distribute by Email to the members on the mailing list (about 700 world wide) information which is of interest to our members. If you have information which you would like sent

### 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/45 directory:       | cd ccp5.newsletters/45          |
| 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                            |

#### 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.

Post-doctoral and lectureship vacancies

Doctoral studentship vacancies

out in this way please send Email to M. Leslie. We also send out post-graduate, post-doctorate and lectureship positions notified to us. Normally post-graduate positions within the UK only are advertised in this way and the Email is 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.

## 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).

Version 1.5 and 1.6 of Shell-Dynamo are now available by anonymous ftp from `hp2.kosmos.keele.ac.uk` (160.5.15.131) in `pub/dynamo/shell1.6.tar.Z`. Alternatively you can obtain it via WWW using the first URL below.

Details of the release are appended

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Telex: 36113 UNKLIB G

URL (professional)  
URL (personal)

[http://www.keele.ac.uk/depts/ph/tc/cph\\_hme.html](http://www.keele.ac.uk/depts/ph/tc/cph_hme.html)  
<http://www.keele.ac.uk/depts/ph/fincham/home.html>

### Changes from Version 1.4

There is an alternative representation for the short-range repulsive potential, of the form  $(A/r) * \exp(-r/\rho)$  instead of the usual  $A * \exp(-r/\rho)$ . This gives greater anharmonicity. It can be used in conjunction with the breathing shell model. See command ERISINT. The breathing shell model can also have an anharmonicity parameter.

It is also now possible to use tabulated short-range interactions (commands TABINT and INTVAL)

A utility program `tabulate` can produce tabulated potentials of the general  $\exp(-6)$  form, but with some methods for fixing up the black hole at the origin.

The documentation now points out that the  $D/r^8$  term in the potential is NOT implemented in the force routine.

There was a bug in the force routine which resulted in inaccurate forces at very large shell-core separations. This circumstance is unlikely to arise, but it has been corrected. To correct version 1.4 replace, in the file `forces.f`, the line

```
if (alphar.gt.0.01) then
```

by

```
if (alphar.gt.0.1) then
```

Other minor corrections include an error in the STATE AVBOX command, and in some instances an incorrect volume being set if UNITCELL was followed by FILLBOX.

See file "outline" for outline documentation

See file "commands" for command language details.

This program is copyright, (C) 1995 David Fincham. You are encouraged to make free use of

it for academic purposes subject to the terms of the free academic licence in the file "licence".

## REQUEST FOR CONTRIBUTIONS

Contributors to the current issue

Our thanks go to:

|                         |  |
|-------------------------|--|
| D. B. Nicolaides        | Department of Chemical Engineering<br>University of Bradford<br>Bradford BD7 1DB, U.K. |
| M. Gillan<br>D. Fincham | Physics Department<br>Keele University<br>Keele, Staffordshire<br>ST5 5BG, U.K.        |
| W. Smith<br>M. Leslie   | CCLRC Daresbury Laboratory<br>Daresbury, Warrington<br>Cheshire<br>WA4 4AD U.K.        |

The deadline for contributions for the next 2 newsletters will be **1 August 1996 and 1 November 1996** Readers are reminded that contributions are always welcome. 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   | m.leslie@dl.ac.uk |
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## MEETING AND WORKSHOP ANNOUNCEMENTS

### CONDENSED MATTER SIMULATION REALIZING THE POTENTIAL OF THE COMPUTER

Churchill Hall, University of Bristol  
23–25 September 1996

The Annual Conference of CCP5<sup>†</sup> will take place at Churchill Hall, University of Bristol, from Monday 23 to Wednesday 25 September 1996. All areas of condensed matter simulation will be represented. The theme of the meeting will be the practical exploitation of the power of computer simulation in the fields of pure and applied research into condensed matter.

Many different approaches, from ab initio molecular dynamics to mesoscopic lattice models, are used to simulate condensed matter systems. In this rapidly-evolving field, cross-fertilization of ideas and techniques is vital. This conference provides an opportunity for experts within the UK simulation community to interact with each other, with representatives of UK industry, and with a number of visitors from overseas.

Invited speakers confirmed to date include:

- P. Cordero (Santiago, Chile)
- B. Dünweg (Mainz, Germany)
- M. Ferrario (Modena, Italy)
- J. Joannopoulos (MIT, USA)
- B. Smit (Shell, Amsterdam)
- M. Stoneham (UCL, UK)
- S. Toxvaerd (Copenhagen, Denmark)

The meeting will start at 9:00 a.m. on the morning of Monday 23 September (accommodation on the Sunday night will be provided) and will finish at lunchtime on Wednesday 25 September.

Registration information, and a general invitation to contribute talks and posters, will be made available shortly. For current information please see the CCP5 World Wide Web server:

*<http://www.dl.ac.uk/CCP/CCP5/main.html>*

<sup>†</sup> This conference is organized under the auspices of the Engineering and Physical Sciences Research Council Collaborative Computational Project # 5, on Condensed Matter Simulation.

## **The 3rd International Conference on Computer Simulation of Radiation Effects in Solids**

University of Surrey, Guildford, UK  
22-26 July 1996

Editors note - The details of this conference have already been distributed by Email; a summary is included here for the benefit of readers who receive paper copies of the newsletter.

### **Scope of the Conference**

The International Conference on Computer Simulation of Radiation Effects in Solids (COSIRES'96) addresses the application of computer simulation methods to the study of the interaction of energetic particles with materials. It offers a forum for the presentation of the latest results and technique developments in this growing field of research. In recent years both the availability and power of computers has increased enormously, many developments have been made in producing more physically meaningful simulations of this subject. Topics will include:

|   |  |
|---|--|
| Interatomic Potentials & Simulation Methods | Low Energy Ion Beam-Surface Interaction    |
| Electronic Energy Loss                      | Plasma Processing of Materials             |
| Electron-Phonon Coupling                    | Electron and Laser Interaction with Solids |
| Radiation Damage and Cascade Effects        | Comparisons of Models to Experiments       |
| Calculations of Implantation Phenomena      | Simulation of Ion Beam Analysis Tools      |
| Energetic Cluster Impacts with Surfaces     | Animation and Visualisation Techniques     |
| Sputtering                                  | Particle Surface Interactions              |
| Ion Beam Mixing                             | Radiation Effects in Biological Materials  |

For further information please contact

Karen Arthur  
Conference Secretary, COSIRES'96  
Department of Electronic & Electrical Engineering,  
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UK  
email: K.Arthur@ee.surrey.ac.uk  
fax: +44 (0)1483 34139  
<http://www.ee.surrey.ac.uk/COSIRES>

## 2nd European Cray MPP Workshop

A two-day workshop hosted by the Edinburgh Parallel Computing Centre and supported by the UK's High Performance Computing Initiative and Cray UK.  
25-26 July 1996

### Introduction

This meeting follows on from the very successful 1st European Cray T3D Workshop held by EPFL in Lausanne in September 1995. The workshop is intended for computational scientists and engineers working in applications development, systems administration or software support for Cray MPP systems (T3D's and T3E's) installed in Europe.

### Talks and Posters

Anyone interested in making a presentation or poster on any of the following topics should indicate their Topic / Title on the registration form.

Applications in Science and Engineering  
Cray MPP Systems Management

Programming Models  
Performance Optimisation

Since time constraints limit the possible number of talks, we will have poster sessions in the conference foyer. The closing date for speaker registration is 17 May 1996; the programme will be circulated in late May.

### Fees

There are no fees for attending the conference. Coffee and lunch will be provided, but all other expenses must be paid by the participants.

### Details

The workshop will take place in the James Clerk Maxwell Building, The King's Buildings, Edinburgh, Scotland on 25-26 July 1996. The first session will start at 10:00, and the workshop will end by 17:00 on the second day.

The programme of talks will be selected by the Organising Committee. This is chaired by David Henty and comprises Stephen Booth, Caroline Neave and Alan Simpson from EPCC; Rob Allan from the Daresbury Laboratory; Zdenek Sekera from Cray Research Switzerland (CRAY-EPFL PATP project).

Further information on the background to this workshop is available.

## **Accommodation**

Accommodation is extremely difficult to find in Edinburgh during the tourist season. We have pre-booked a number of rooms in convenient, low-cost accommodation at Pollock student halls of residence (the location is shown on the city centre map). The charge is 30 pounds per night for bed-and-breakfast and includes bus transport to the workshop. These rooms will be offered on a first-come first-served basis.

If you want to be sent an accommodation form, please indicate on the registration form. We think you will find it easier to use the accommodation we have arranged, and we urge you to register early as the number of rooms available is limited. However, if you prefer to make your own arrangements you can consult our accommodation list.

## **Travel**

Edinburgh is easily accessible by air, rail and road. We have maps of the city and the King's Buildings campus.

## **Registration**

Those wishing to speak and/or attend are invited to fill in the registration form. The deadline is 17 May if you want to give a presentation, 31 May otherwise. If you experience any problems registering, please email [workshop@epcc.ed.ac.uk](mailto:workshop@epcc.ed.ac.uk).

# **PHYSICS COMPUTING'96**

Krakow, Poland  
17-21 September 1996

Editors note - The details of this conference have already been distributed by Email; a summary is included here for the benefit of readers who receive paper copies of the newsletter. Full information about this meeting may be found at URL <http://www.cyf-kr.edu.pl/pc96>

## **Organizing institutions**

The Conference is organized jointly by:

Academic Computer Centre CYFRONET - KRAKOW, Krakow, Poland  
Interdisciplinary Group on Computational Physics of the European Physical Society  
under the auspices of the European and the American Physical Societies.

### **Important dates**

|                   |  |
|-------------------|--|
| 10 May 1996       | deadline for receipt of contributed papers |
| 31 May 1996       | notification of acceptance of papers       |
| 15 June 1996      | deadline for registration with reduced fee |
| 17 September 1996 | PC'96 Conference                           |

### **Scientific Program**

PC'96 Conference will be a forum for physicists throughout the world for whom the COMPUTER is the MAIN TOOL of RESEARCH. We hope that Conference will enable them to exchange ideas and research results relating to the fast-growing field of computational physics and to share experience with the most advanced developments in computer hardware and software. The scientific program of the conference will consist of invited lectures, contributed oral presentations, classical and virtual poster sessions, tutorials and vendor presentations.

### **Main topics of the meeting**

Main topics of the meeting will cover:

|  |   |
|--|---|
| various fields of computational physics, such as | as well as contemporary trends in hardware    |
| computer simulation in statistical physics       | and software development:                     |
| simulation of specific materials                 | recent developments in computer architectures |
| surface phenomena                                | modern programming techniques (parallel       |
| percolation                                      | programming, object oriented approach)        |
| critical phenomena                               | symbolic computations                         |
| computational fluid dynamics                     | graphics, visualization and animation         |
| classical and quantum molecular dynamics         |   |
| chaos dynamical systems                          | together with industrial applications and     |
| self-organization and growth                     | teaching of computational physics.            |
| neural networks and their applications           |   |
| complex optimization                             |   |

### **Invited lectures**

This is a partial list of those of most interest to CCP5, for a complete list refer to the URL given above.

|                       |  |  |
|-----------------------|--|--|
| Kurt Binder           | University Mainz,<br>Germany                 | Large scale Monte Carlo simulations: a powerful tool for material science? |
| Janos Kertesz         | Technical University of<br>Budapest, Hungary | Computer simulation of surface growth                                      |
| Peter Lomdahl         | Los Alamos National<br>Laboratory, USA       | Large scale molecular dynamics on MPPs                                     |
| Mike Payne            | Cavendish Lab.,<br>Cambridge, UK             | Ab initio total energy pseudopotential calculations                        |
| Dennis C.<br>Rapaport | Bar-Ilan University,<br>Ramat-Gan, Israel    | The art of molecular dynamics simulation                                   |

Up-to-date list of invited lectures is on the PC'96 www pages.

PC'96 www pages also has information on

|                        |           |                   |               |
|------------------------|-----------|-------------------|---------------|
| Registration Fees      | Tutorials | Papers Submission | Accommodation |
| Time schedule of PC'96 |           | Social program    | Payment       |

### Further Information

For more information about PC'96 contact:

|   |  |
|---|--|
| <a href="http://www.cyf-kr.edu.pl/pc96">http://www.cyf-kr.edu.pl/pc96</a> | Marian Bubak                               |
| <a href="ftp://ftp.cyf-kr.edu.pl/pc96">ftp://ftp.cyf-kr.edu.pl/pc96</a>   | Physics Computing 96                       |
| <a href="mailto:pc96@cyf-kr.edu.pl">email:pc96@cyf-kr.edu.pl</a>          | Academic Computer Centre CYFRONET - Krakow |
|   | P. O. Box 386                              |
| Phone: (48 - 12) 341 766; 173 964   | Nawojki 11                                 |
| Fax: (48 - 12) 341 084; 338 054   | 30-950 Krakow 61                           |
|   | POLAND                                     |

## Optical, electric and Magnetic Properties of Molecules

Cambridge University, UK  
10-13 July 1997.

Editors note - The details of this conference have already been distributed by Email; a summary is included here for the benefit of readers who receive paper copies of the newsletter.

This conference is being organised to celebrate the career of Professor A. David Buckingham. Those interested in being placed on the mailing list should contact

Professor David C Clary,  
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**The Royal Society of Chemistry  
FARADAY DIVISION**

**Divisione di Chimica Fisica, Societa' Chimica Italiana  
Deutsche Bunsen Gesellschaft für Physikalische Chemie  
Société Française de Chimie, Division de Chimie Physique**

Faraday Discussion No: 106  
Solid State Chemistry: New Opportunities  
from Computer Simulations

University College, London  
30 June - 2 July 1997

**ORGANISING COMMITTEE:**

Professor C R A Catlow  
Dr N L Allan  
Dr S L Price

AND

Dr W C Mackrodt (Co-Chairman)  
Professor P W Fowler  
Dr P A Madden

Over the past decade or so, one of the major developments in chemistry has been the increasingly important role played by high performance computing. Nowhere is this more evident than in solid state chemistry, where computer simulations are now a major source of understanding and interpretation and the generator of data which is either difficult or impossible to obtain by other means. The Discussion will highlight recent developments with a view to assessing likely directions for the future.

The meeting will embrace:

*ab initio* electronic structure methods  
lattice statics and dynamics  
molecular dynamics  
Monte Carlo simulations

Systems for discussion will range in complexity from simple solids to high Tc superconductors, catalysts, microporous materials, molecular solids, glasses and fullerenes including surface properties and reactivity.

Contributions are invited for consideration by the Organising Committee. Titles and abstracts of about 300 words should be submitted no later than FRIDAY 26 JULY 1996 to Dr W C Mackrodt, School of Chemistry, University of St Andrews, Fife KY16 9ST.

Full papers for publication in the Faraday General Discussion 106 volume will be required by February 1997.

Updated conference information may be found on WWW at this URL: <http://chemistry.rsc.org/rsc/farad106.htm>

## Chemical Database Service

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Telephone +44 (0)1925 603162  
E-mail cdsbb@dl.ac.uk  
May 1996

### The Chemical Database Service

Daresbury Laboratory provides a Chemical Database Service to the UK academic community. The aim of the service is to ensure that the growing body of information from chemistry research is conveniently accessible to the UK academic community in ways which foster the essential UK core competency in Chemistry. This is done by providing on-line access via Internet to a range of databases in the areas of crystallography, synthetic organic chemistry, spectroscopy and physical chemistry - see below. Three chemists provide help, support and advice to users of the service.

### Components Presently Available

**CSD** The Cambridge Structural Databank. Crystal structure data for over 152,000 organic and organo-metallic compounds. Two releases of this databank are received and mounted annually (April and October). QUEST has 3D search capabilities.

**ICSD** Inorganic Crystal Structure Data File. Over 40,000 inorganic structures - the companion file to the Cambridge organic file (though in a different format).

**MDF** Metals Data File. Crystal structure data for over 55,800 metals and alloys.

**PDB** The Brookhaven Protein Data Bank containing bibliographic and coordinate details for over 4,400 proteins and other biological macromolecules.

**CDIF** Crystal Data Identification file. Crystal class and unit cell data for over 210,400 crystal structures.

**FNMR** A databank of about 6,000 <sup>19</sup>F NMR spectra and coupling constants.

**ELYS** Electrolyte Solutions Database. Thermodynamic and transport property data such as density, viscosity, diffusion coefficients etc. Currently contains about 10,000 entries.

**ISIS/REACCS** Chemical reaction information management systems allowing search, retrieval and display of molecules, reactions and their associated data. ISIS is a client/server system

and is the replacement for REACCS. Currently ISIS can access over 605,000 searchable reactions and REACCS 240,000, from the following databases:

**THEILHEIMER** (Synthetic Methods of Organic Chemistry)

**CHC** (Comprehensive Heterocyclic Chemistry)

**CLF** (the Current Literature File)

**CHIRAS** (Asymmetric Synthesis)

**METALYSIS** (Transition metal-mediated transformation)

**REACCS-JSM** (Journal of Synthetic Methods)

**CHEMINFORM** (current awareness) only available via ISIS

**CSM** (Current Synthetic Methodology) a subset of CHEMINFORM, only available via REACCS

**ORGSYN** (Organic Synthesis) only available via ISIS

**ORAC CORE** (Established Literature) only available via ISIS

**SPG** (Protecting Groups) only available via REACCS

ISIS also allow access to ACDRX (Available Chemicals Directory), which is a database of suppliers of chemicals. It contains over 180,000 different compounds.

**SPEC** SpecInfo is a multi-technique spectroscopic database system which will cover NMR, IR and mass spectra. The package is designed to aid the chemist in spectral interpretation and structure elucidation problems. It contains spectral data sets with their associated structure connection tables. The database currently contains 72,000 <sup>13</sup>C, <sup>15</sup>N, <sup>17</sup>O, <sup>19</sup>F and <sup>31</sup>P NMR spectra and 20,000 infra-red spectra.

A variety of utility programs are also available, including chemical file format conversion, molecule viewers, gopher and World-Wide-Web browsers.

For further information contact:

Chemical Database Service  
Room C18, Daresbury Laboratory  
Daresbury, Warrington  
WA4 4AD  
Tel: (01925) 603162  
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## Report of the visit of Ronald Cohen to the UK

Ronald Cohen  
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November 16, 1995

Thanks to partial support from CCP5 I was able to visit University College London, University of Cambridge, and Oxford University to present a series of seminars, exchange ideas, and form the basis for future collaborations.

I first attended the workshop “Developments in Mineral Physics–Collective Phenomena”, a workshop in honor of Professor Desmond McConnell at Darwin College. Here is a brief summary of that meeting.

Professor McConnell (Oxford) first summarized several years of work on the nature of H and H<sub>2</sub>O in quartz (SiO<sub>2</sub>). It is well known experimentally that H<sub>2</sub>O greatly weakens (lowers the shear strength of) quartz, and that H<sub>2</sub>O greatly enhances diffusivity of O (measured via isotope experiments), but the microscopic reason was not previously understood. First principles calculations with Professor V. Heine and others showed that the hydrolytic weakening can be quantitatively understood in terms of depolymerization of the quartz structure by the formation of H<sub>4</sub> defects that aggregate together to form H<sub>2</sub>O islands when a crystal is strained. These islands also become weak points for failure. The effect of H<sub>2</sub>O on isotope exchange rates can be understood by the diffusion of H<sub>2</sub>O into the channels in quartz, followed by exchange between the O in the channel water and the bulk. Large scale computations for supercells within the LDA and plane wave pseudopotentials gave good estimates of the relative energetics of different H and H<sub>2</sub>O defects compared with calorimetry and T-dependent experiments.

Dr. Ross Angel (Bayreuth) gave a summary of recent work on isosymmetry phase transitions, especially recent work he has done on pyroxenes and feldspars. Within the resolution of the experiments, behavior is observed that is similar to that seen in displacive phase transitions, which usually involve changes in symmetry. Over a limited range of T or P, structural parameters vary rapidly, and very often P-T boundary bend sharply in the vicinity of one of these transitions. The phases are often structurally distinct, in spite of having the same space group symmetry. In the pyroxene example, one C2/c “phase” has kinked chains, whereas the other has straight chains. Other examples were discussed, including KTP, Ce, and H<sub>2</sub>O.

Professor Volker Heine (Cambridge) gave an overview of a number of current research projects. M.H. Lee is working on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, which is an fcc structure with disordered occupancies of T and O sites. They found that empirical potentials gave the wrong energy differences between the T and O sites, so LDA pseudopotential calculations are being performed. M. Gambhir is working

on short range order in cristobalite. A. Pryde is studying diffuse scattering in low-tridymite from Rigid Unit Modes (RUM's). K. Hammonds is studying floppy modes in zeolites. R. Shav is using first-principles methods to study the reaction  $\text{methanol} + \text{H}^+ \rightarrow \text{CH}_3^+ + \text{H}_2\text{O}$ , where the reaction is catalyzed by a zeolite, chabazite, which also provides the  $\text{H}^+$ . They are finding that a floppy mode is important to bring the  $\text{H}^+$ 's to the  $\text{CH}_3\text{OH}$ . Collaborations with Dr. M. Dove (Cambridge) involve studying Si-Al ordering using different order-disorder models.

In collaborative work in Professor Salje (Cambridge) Professor Heine also discussed the origin of tweed textures and how almost any non-equilibrium perturbation can cause tweed to set in when there are long-range elastic forces.

Professor Salje continued the discussed of tweed textures and discussed how new rocking geometry diffractometers at Cambridge are being used to map out the diffuse scattering due to twins, tweed, etc., and are being used to quantitatively describe the behavior.

Dr. R. Cohen (myself) gave an overview of research at the the Geophysical Laboratory (GL) using three different approaches 1) all-electron, full-potential LAPW (Linearized Augmented Plane Wave) computations within the LDA and GGA, 2) much faster Gordon-Kim like models, such as the VIB (Variationally Induced Breathing) model for ionic solids such as  $\text{MgO}$ , and 3) a new tight-binding total energy model which has accuracy rivalling that of the FLAPW when the model is used within the sphere of its parameterization, but which is many hundreds of times faster. Examples were given of studies using the different methods, and collaborative work with experimentalists at the Geophysical Lab were discussed. LAPW calculations on  $\text{SiO}_2$  stishovite predicted a phase transition to the orthorhombic  $\text{CaCl}_2$  structure at 45 GPa. High pressure Raman experiments at GL that showed the  $B_{1g}$  mode stopped softening at 50 GPa and begins to harden, in excellent agreement with predictions. LAPW calculations on  $\text{FeO}$  explain the origin of the observed rhombohedral strain and predict a loss of local magnetic moments with increasing pressure. The advantage of the VIB model is that long MD trajectories can be studied without sacrificing accuracy, at least for  $\text{MgO}$ . Recent equation of state studies (Inbar and Cohen) were discussed that show excellent agreement with the thermal equation of state. Melting of  $\text{MgO}$  was studied using both clusters (Cohen and Gong) and periodic boundary conditions (Cohen and Kluge) and obtain similar results, in disagreement with recent experiments (Zerr and Bohler) but consistent with systematics of alkaline earth oxides. Thermal conductivity simulations were mentioned. A new tight-binding total energy model (TBTE) was briefly discussed, and results were shown for Fe and Xe. The model accurately predicts properties over wide ranges of compression (within the bounds of the fit) and is being used for finite T simulations. The parameters are fit to LAPW total energies and band structures.

Dr. P. Ballone (MPI Stuttgart) discussed plane-wave pseudopotential simulations for three geophysically important polymorphs of  $\text{Mg}_2\text{SiO}_4$ , olivine (Pbnm, 28 atoms/primitive cell),  $\beta$ -spinel (Imma, 56 atoms/cell), and spinel (Fd3m, 14 atoms/cell) performing relaxations and studying the equations of state and phase transitions. Results are quite accurate. The olivine spinel transition is given at 12 GPa compared with 10 experimentally. He also discussed H in  $\text{Fe}_2\text{SiO}_4$  (fayalite) and liquid fayalite which is an antiferromagnetic liquid. First-principles simulations were performed for 0.15 psec at 1800 K for 112 atoms. The difficulty of doing long trajectories with first-principles

(i.e. self-consistent) methods was pointed out.

Dr. W. Schranz (Vienna) discussed recent progress on the central peak problem. He showed new results on homogeneous and inhomogeneous elastic measurements. He discussed different origins of central peak phenomenon, but concentrated on entropy fluctuations (heat waves) near phase transitions and gave a series of models to explain the observations. Extensive discussions were given of elastic and dielectric behavior near phase transitions, and gave an understanding of strong dispersion in elasticity observed around ferroelastic phase transitions.

Dr. D. Sherman (Bristol) discussed Hartree-Fock periodic CRYSTAL calculations of H<sub>2</sub>O in diaspore, boehmite ( $\alpha$ -AlOOH,  $\gamma$ -AlOOH) and brucite (Mg(OH)<sub>2</sub>). He obtained deep potential wells for the H's, and claimed that tunneling is important even though the wells were 1 eV deep. He studied the equation of state of brucite and says that quantum delocalization sets in at high pressures. His conclusion was that there isn't much water in the Earth.

After the meeting, I traveled to University College London and presented a departmental seminar on similar topics to the above, but with the addition of recent work on the Earth's core. A combination of LAPW and TBTE calculations have been used to study the thermal equation of state and elasticity of Fe under core pressures. This work has been done in collaboration with Lars Stixrude and Evgeny Wasserman at the Ga. Inst. Technology. We find excellent agreement with seismological and free oscillation observations of anisotropy in the Earth's inner core if the inner core contains a huge single hcp crystal oriented approximately with the c-axis along the Earth's rotation axis.

At UCL I had extensive discussions with Professor D. Price and members of the department, including Drs. L. Vocadlo, J. Brodholt, N. Ross, and A. Patel. A. Patel et al. performed simulations of the thermal equation of state of MgSiO<sub>3</sub> perovskite. Vocadlo and Price have studied melting of MgO at high pressures using the THB2, Matsui, and Lewis and Catlow empirical potentials, and their results are almost identical to those we obtained recently (Cohen and Kluge) using the VIB model. We also discussed the melting of perovskite. We plan to form an active collaboration, and Dr. Vocadlo will visit GL for collaborative work. Discussions with Drs. J. Brodholt and N. Ross centered on the reported "kinks" (Chopela and others) in Raman frequencies versus pressure in olivine and perovskite.

On October 26 I presented a seminar for the TCM group at Cavendish on first-principles studies of ferroelectrics, and discussed work done at GL on bulk and slab BaTiO<sub>3</sub>, PbTiO<sub>3</sub>, LiNbO<sub>3</sub>, and LiNbO<sub>3</sub>. The goal is to understand the origin of ferroelectric behavior, the reasons for different behavior in similar materials, and the differences between the perovskite and LiNbO<sub>3</sub> families. I had extensive discussions with Dr. C. Molteni about first-principles simulations of grain boundary sliding and with N. Marzari on linear response computations for solid solutions, as well as with others.

On October 27 I gave a seminar for the Materials Department at Oxford on the new TBTE model and discussed applications to high pressure research. I visited the Modeling Laboratory and had extensive discussions with Dr. A. Bratkovsky on bond-order potentials and order N methods as well as with others.

On October 30 I gave a seminar at the Earth Science Department at Oxford primarily on Fe in the Earth's core, and discussed in more detail the computations on Fe, the evidence that the inner core is largely a single crystal, and an overview of the geophysics of the core. I had extensive discussion with Dr. A. Jephcoat, and we have started two exciting collaborative theory and experimental projects on  $\text{AlH}_3$  and  $\text{LiNbO}_3$  at high pressures. I also had discussions with Prof. D. McConnell on effects of water on feldspar order-disorder, and extensive talks with Dr. K. Refson on LDA plane-wave pseudopotential methods and comparison with all-electron results and Hartree-Fock, which will probably lead to collaborative research and joint code development.

All in all it was a very fruitful scientific trip, and it is great that CCP5 can help bring such exchanges about. I should acknowledge my collaborators: B. Burton, Z. Gong, I. Inbar, D. Isaak, M. Kluge, I. Mazin, F. Marton, L. Stixrude, and E. Wasserman. I also thank the National Science Foundation, the Office of Naval Research, and the Carnegie Institution of Washington for supporting my research.

## **Report of Visit to UK by Professor Stefan Estreicher (Texas Tech University)**

19-25 March 1996

### **Visit to London by Professor Stefan Estreicher**

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In the London part of his trip, Professor Estreicher visited the Condensed Matter and Materials Physics group at University College London. He gave a talk on "Passivation processes in silicon" on 25 March, which was attended by an audience of about thirty people. The audience was drawn from the group at University College, from the Physics Department at King's College, from the Semiconductor IRC at Imperial College, and from the Rutherford Appleton Laboratory.

There was a lively discussion at the seminar and over the lunch following, which focussed (among other things) on

1. The role of basis-set superposition error in electronic structure calculations of defects;
2. The importance of zero-point energy in the free energies of defects involving light interstitials (particularly hydrogen);
3. The possible identity of rapidly-diffusing passivating species which are implied by recent developments in solar cell technology;
4. The candidate structures for various defect-hydrogen complexes, and their possible uses in passivation.

### **Visit to Edinburgh by Professor Stefan Estreicher**

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Prof Eistreicher spent two days with us in Edinburgh, speaking with all members of the Condensed Matter Group involved with solid state simulation. We had very helpful discussions regarding the mechanism for neutral self-interstitial diffusion in silicon, a topic of mutual interest, and he had some interesting observations to make regarding our discovery of threefold rings of carbon atoms in amorphous carbon, in particular on the possibility that they might be remnants of  $C_3$  clusters (stable as equilateral triangles) from the high temperature starting phase. His talk, on work carried out some time ago regarding diffusion in silicon, but excluding his very recent discoveries of hydrogen enhanced diffusion of oxygen, was delivered to a small audience of about 20.

Although, in the event, I was unable to arrange the good weather I had promised, Prof. Eistreicher also enjoyed a few days of being a tourist in Edinburgh. We also invited Stefan to a group meal which was well enjoyed by all, even the haggis pizza. The whole group found Prof Eistreicher's work of interest and him very approachable. In all it was a very successful visit, both scientifically and socially, and I should like to thank CCP5 for making it possible.

## Report on CCP5-sponsored visit to UK of Professor Martin Schoen (TUB Berlin)

Professor Schoen visited the Department of Chemistry, University of Manchester, where his host was Dr. Andrew Masters; the Department of Chemistry, Imperial College London, hosted by Professor Dominic Tildesley; and the Department of Physics, University of Bristol, where his host was Dr. Mike Allen.

Martin arrived at Manchester from Berlin via Frankfurt on the morning of Tuesday 7 May. The journey was slightly jeopardized by the recent fire at Dusseldorf, which had made the originally scheduled route impossible; the revised connection at Frankfurt turned out to be very tight.

Martin mainly talked with Andrew Masters, his post-doc., Lena Akhmaskaya, and Julian Clarke from UMIST, with whom he shares many common simulation interests. He gave a seminar entitled *Phase transitions in confined films. Computer simulations and theoretical results* which covered shear-induced melting of confined solids, the microscopic structure of a near-critical fluid in a pore and some beautiful work on layering transitions in confined geometries. On Wednesday, Martin departed by train for London.

Martin arrived in London at about 5.30 p.m. on 8th May. We were able to find him accommodation in one of the Imperial College Guest rooms in Prince Consort Road just opposite the college. Ian Gould and David Nicholson took Martin to dinner at the Brasserie St Quentin in Knightsbridge, ensuing an auspicious start to his visit

We worked hard on the Thursday. Martin spent the first hour with Dominic Tildesley. They discussed Dominic's recent work on the calculation of the non-linear susceptibility and modelling of the second harmonic generation at the air/water interface and studies of flexible molecules dissolved in the Gay Berne fluid. Martin described his recent work on diffusion in confined monolayer films and a Taylor series Monte Carlo simulation method, which is reminiscent of the multiple time-step methods in molecular dynamics.

After coffee, Martin spent time with David Nicholson. David discussed his recent work on grand canonical simulations of mixtures in pores, his molecular dynamics studies of self-diffusion in slit geometries and new intermolecular potentials for zeolites. We introduced Martin to Dr Julian Gale, our Royal Society Research Fellow. Julian described his work based on the first density functional calculations of molecular adsorption on zeolite fragments. Recently this area has been extended to the use of plane-wave methods to study the binding of adsorbates in a periodic representation of a micro porous material.

We went to the Imperial College staff canteen for lunch and to take our mind off the food, we discussed the changes in Berlin since reunification. It is always a great pleasure to swap stories on the government's unusual approach to managing academic affairs. The chaos stretches across Europe.

In the afternoon Martin had an opportunity to meet the post-doc's and graduate students. He had an interesting session with Vladimir Sokhan discussing the adsorption of phenol at a water liquid/vapour interface and with Patrick Harvey on the penetration of oil into surfactant layers.

Martin was full of ideas and questions and I think this session was enjoyed by all. We remembered to give him some time to think about his own talk and we had arranged tea for 4.00 pm in the old part of the Chemistry Building, which houses some magnificent Victorian lecture theatres.

We enjoyed an excellent seminar. Martin's observations on the significant changes in the lateral liquid structure of a fluid during pore filling gave rise to a large number of questions about the order and nature of the underlying phase transition. The seminar was much appreciated by a small but well-informed audience.

After a vote of thanks, we gave Martin a short seminar on the vagaries of the London Underground and delivered him with clear instructions for Paddington by way of South Kensington.

Martin arrived in Bristol shortly after 9 p.m., and had dinner with Mike Allen at Browns Restaurant, recently converted from the University Student Refectory into a place that serves decent food. An early start the next day saw Martin in detailed discussions with Mike and his students. Philip Camp described recent simulations of biaxial nematic ordering in rod-plate mixtures, and the mapping out of the isotropic-nematic coexistence line for uniaxial hard ellipsoids by Gibbs-Duhem integration. This work is directly connected with testing recent improvements to the classical Onsager theory. Julian Brown outlined work carried out in collaboration with the group in Seville, investigating the effect on the phase diagram of systematically varying parameters in the Gay-Berne model. Martin has recently begin work on the effects of confinement and simple models of molecule-surface interaction on this type of model, and there seems to be some scope for collaboration and exchange of information in the future. Mike Allen also described recent determinations of the Frank elastic constants for this system by his student Mark Warren. Martin spent some time discussing a range of simulations with Jeroen van Duijneveldt, a Ramsay Research Fellow in the group.

With Bob Evans, Martin discussed theoretical aspects of the effects of confinement on phase transitions, some of the related experimental work going on in the laboratory in the group of Ashraf Alam, and the effect of the long-range form of the pair potential on the asymptotic form of pair correlation functions and density profiles. With Bob, Mike Allen and Hector Dominguez, he discussed some simulation work of Hector's on the effect of confinement on the freezing transition, which involves some quite delicate free energy calculations.

The seminar was quite well attended, provoked much discussion, and was appreciated by all. Afterwards, Martin had the chance to talk to Margarita Rivera, a graduate student in the polymer group, who has performed a range of experiments on complex molecules adsorbed on surfaces using STM/AFM apparatus.

On Saturday, some time was devoted to tourism. Mike and Martin started by giving moral support to Philip Camp, who was playing in a two-day croquet tournament (more hard-particle dynamics). Then a guided tour of Bristol, part on foot, part by boat, followed. After lunch, Mike went home to watch the FA Cup Final on television, while Martin slept back at the University accommodation; it is debatable who had the more interesting time. A final dinner at the local Balti restaurant brought the visit to an end. Martin departed very early next morning for Heathrow by coach.

All those involved thought the visit worthwhile. Our thanks go to Martin Schoen for undertaking such a tour, talking to so many people, and being so interested in everything he encountered. CCP5 would like to thank the institutions who cooperated in this venture.

## Book Review

The Art of Molecular Dynamics Simulation  
by D. C. Rapaport  
Cambridge University Press, 1995, £45 (hardback)  
ISBN 0 521 44561 2

The author describes this as an introductory text, a recipe book, and a reference manual. The title recognises that simulation, like cooking, is as much an art as a science.

The approach is, within each chapter, to develop theory and methodology together, usually followed by examples and exercises. Algorithms are described using program listings which are integrated into the text, and it is this feature in particular which gives the book its practical flavour which will be much appreciated by beginners.

After an introductory first chapter the author devotes four chapters to developing the fundamental methods used to study simple fluids. Topics discussed are force evaluation, including neighbour list and cell search methods; leapfrog and predictor-corrector integration schemes; measurement of thermodynamic and structural properties (including Voronoi polyhedra); transport coefficients; and dynamic structure factors. There are then chapters on constant temperature and constant pressure methods, and on non-equilibrium methods, before the author turns to molecular systems. Rigid molecule dynamics is described using a quaternion representation with a predictor-corrector algorithm; flexible molecules are also discussed, including the use of angle and torsion forces and the application of bond-length constraints. The next chapters cover the Ewald sum (applied to dipolar systems); three-body forces; and hard-sphere simulations. Finally there are two chapters which reflect particular research interests of the author: on the atomistic approach to fluid dynamics; and on algorithms for parallel and vector supercomputers.

The treatment is thorough and the style readable. A student who works through this book will gain an excellent grounding in molecular dynamics simulation. As a reference manual it is perhaps less successful, since its very thoroughness necessarily leads to omissions. Some of my favourite algorithms are missing (leapfrog rotational algorithms, loose coupling thermostat and pressurestat) and a weakness is the lack of consideration given to ionic materials.

An aspect of the book that will be controversial is the choice of the C language for the program listings. The author has avoided the use of C features that are not found in Fortran 77 but some will feel that he thereby ends up with the worst of both worlds. To keep the listings short he makes liberal use of global variables (which are listed in an appendix): a bad habit to encourage.

The book invites comparison with those by Allen and Tildesley (ISBN 0 19 855375 7) and Haile (ISBN 0 471 81966 2). Allen and Tildesley cover much more ground, with a deeper theoretical basis, more algorithms (including Monte Carlo) and more physical examples, but are less good on implementation details. Haile covers a few methods at a deep, almost philosophical, level but fails to get beyond the soft-sphere model, and relegates programming considerations to an appendix. Allen and Tildesley remains a very useful reference, Haile can be read with profit by beginners and experts alike, but Rapaport has provided the best introductory text.

David Fincham