

CCP3

SURFACE

SCIENCE

NEWSLETTER

Collaborative Computational Project 3
on Surface Science

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Contributions to the newsletter from all CCP3 members are welcome and should be sent to ccp3@dl.ac.uk. Useful Links:

CCP3 Home Page <http://www.cse.clrc.ac.uk/Activity/CCP3>

CCP3 Program Library <http://www.cse.clrc.ac.uk/Activity/CCP3+896>

SRRTNet <http://www.cse.clrc.ac.uk/Activity/SRRTNet>

DLV <http://www.cse.clrc.ac.uk/Activity/DLV>

CRYSTAL <http://www.cse.clrc.ac.uk/Activity/CRYSTAL>

CASTEP <http://www.cse.clrc.ac.uk/Activity/UKCP>

Many useful items of software are available from the UK Distributed Computing Support web site, DISCO <http://www.cse.clrc.ac.uk/Activity/DISCO>

Editors: Dr. Klaus Doll and Dr. Adrian Wander, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK

1 Editorial

The renewal of CCP3, which is due in the summer, is on all our minds, and this edition of the newsletter reminds us of our aims and achievements. The flagship project supported by the post-doc is at the heart of the CCP – new programs can be developed which would not get off the ground otherwise. Over the last three years CCP3 has been very lucky to have had Klaus Doll working on the development of analytic gradient methods for the CRYSTAL electronic structure package. This will lead to much more efficient structure optimization, of particular benefit to surface scientists where surface relaxation and reconstructions are so important. Klaus' achievements so far are described in the first article, and it is most satisfactory that tests on the CO molecule and bulk MgO have proved successful. The next step is to build in symmetry, to achieve greater computational efficiency, and then the new code can be released. As the flagship in the renewal proposal, the working group has chosen the development of methods to study the electronic structure and physical properties of large clusters. These clusters themselves possess surface-like properties, but at the same time it is proposed to study their interaction with surfaces. Such systems are a topic of active research for several of the members of the working group, both theoretical and experimental, and it is expected that their expertise will contribute greatly to the success of the project.

Having Adrian Wander as a permanent member of staff at Daresbury supporting CCP3 will lead to very welcome support for the synchrotron radiation community in the development of new surface program packages. In this newsletter he describes developments in SRRTNet, originally an American collaboration for providing support for surface scientists using synchrotron radiation, which is likely to develop into an international collaboration based on the CCP model. Adrian is also in discussion with the Daresbury-based X-ray community with a view to developing new codes for the analysis of near-edge spectra in a wider range of systems than can be tackled at the moment, using the improved self-consistent electron potentials available for complex materials. This work would be based at Daresbury, and will form part of the CCP3 collaboration.

This issue contains short articles on our visitor programme, and by Ally Chan (Nottingham) and Yu Chen (Birmingham) who received student bursaries for participating in ECOSS-18. Please continue to apply for CCP3 support! It is interesting to read in the pieces by Ally and Yu what most impressed them at ECOSS – I was struck by Ally's comment that surface science has broadened to include nanoparticles and nanowires. Just what we thought in our choice of flagship project next time round.

John Inglesfield

2 Scientific Articles

Analytical Hartree-Fock gradients for periodic systems

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We report on the progress of the implementation of analytic gradients in the program package CRYSTAL. The algorithm is briefly summarised and tests illustrate that highly accurate analytic gradients of the Hartree-Fock energy can be obtained for molecules and periodic systems.

Introduction

Computational materials science has been a fast growing field in the last years. This is mainly because methods which were developed earlier (density functional theory, molecular dynamics, Hartree-Fock and correlated quantum chemical methods, Monte Carlo schemes, the GW method, etc) can now be applied to demanding realistic systems due to the increase in computational resources (faster CPUs, parallelisation, cheaper memory and disk space).

CCP3 is a collaboration in the area of surfaces and interfaces where progress depends on an interaction between experimental and theoretical approaches. Therefore, codes which provide a better theoretical understanding are important.

One of the key issues in surface science is the determination of surface structure and adsorption energetics. From the computational point of view, a fast structural optimisation must be possible. Availability of numerical or analytical gradients facilitates finding a minimum energy structure, and availability of analytical gradients can make optimisation algorithms more efficient. As a rule of thumb, analytical gradients are about $\frac{N}{3}$ times more efficient than numerical gradients (with N being the number of variables). Also, for future developments such as finding transition states, gradients are essential.

Analytical gradients in quantum chemistry were pioneered by Pulay who did the first implementation for multicentre basis sets[1]. In many molecular codes based on quantum chemistry methods, analytical gradients are now implemented and gradient development has become an important task in quantum chemistry [2, 3, 4, 5]. Similarly, in solid-state codes such as CASTEP, WIEN, or LMT0, analytic gradients are available. Analytic Hartree-Fock gradients have already been implemented in a code for systems periodic in one dimension [6]. CRYSTAL [7, 8] was born in Turin and is now jointly developed in Turin and Daresbury. CRYSTAL was initially designed to deal with the exact exchange in periodic systems and to solve the Hartree-Fock equations for real systems. With the modern versions of the code, density-functional

calculations or calculations using Hybrid functionals such as B3LYP with the admixture of exact exchange are also possible.

The target of this project, which began in October 1997, was the implementation of analytical gradients in CRYSTAL and in autumn 1999, the first test calculations on periodic systems were performed.

In this article, we try to outline the theory and implementation of analytical gradients. We try to keep the mathematics at a minimum; a more formal publication is intended in the near future[9]. A very comprehensive summary of the theory underpinning CRYSTAL will appear in the future [10].

Total energy

First, we want to briefly summarise how the total energy is obtained. The total energy consists of

- kinetic energy of the electrons
- nuclear-electron attraction
- electron-electron repulsion
- nuclear-nuclear repulsion

CRYSTAL, similar to molecular codes such as GAMESS-UK, MOLPRO (Stuttgart and Birmingham), GAUSSIAN, TURBOMOLE, etc, solves the single particle Schrödinger equation and a wavefunction is calculated. The wavefunction is based on crystalline orbitals $\Psi_i(\vec{r}, \vec{k})$ which are linear combinations of Bloch functions

$$\Psi_i(\vec{r}, \vec{k}) = \sum_{\mu} a_{\mu,i}(\vec{k}) \psi_{\mu}(\vec{r}, \vec{k}) \quad (1)$$

with the Bloch functions constructed from

$$\psi_{\mu}(\vec{r}, \vec{k}) = \sum_{\vec{g}} \phi_{\mu}(\vec{r} - \vec{A}_{\mu} - \vec{g}) \exp(i\vec{k}\vec{g}) \quad (2)$$

\vec{g} are direct lattice vectors, \vec{A}_{μ} denotes the coordinate of the nuclei. ϕ_{μ} are the basis functions which are Gaussian type orbitals. For example, an *s*-type function centred at $\vec{R}_a = (X_a, Y_a, Z_a)$ is expressed as $\phi(\alpha, \vec{r} - \vec{R}_a, n = 0, l = 0, m = 0) = \phi_{\mu}(\vec{r} - \vec{R}_a) = N \exp(-\alpha(\vec{r} - \vec{R}_a)^2)$.

In molecular calculations, no mathematical problem arises from any of the interactions. In periodic systems, however, there are several divergent terms which have to

be dealt with: for example, in a one dimensional periodic system with lattice constant a and n being an index numerating the cells, the electron-electron interaction per unit cell would have contributions like:

$$\sum_{n=1}^{\infty} \frac{e^2}{na} \quad (3)$$

This sum is divergent (similarly in two and three dimensions). Therefore, an individual treatment of this term is not possible. Instead, all the charges (nuclei and electrons) are partitioned and a scheme based on the Ewald method is used to sum the interactions [11].

The Hartree-Fock equations are solved in terms of Bloch functions because the Hamiltonian becomes block-diagonal (i.e. at each \vec{k} -point the equations are solved independently).

The wavefunction coefficients $a_{\mu,i}$ are optimised due to this procedure and the total energy can be evaluated. For the computation of gradients, the dependence of the total energy on the nuclear coordinates must be analysed.

There are three dependencies of the total energy on the nuclear coordinates:

- nuclear-nuclear repulsion and nuclear-electron attraction: obviously, the coordinates of the nuclei enter
- wavefunction coefficients (or density matrix): we will obtain a different solution with different density matrix when moving the nuclei
- basis functions: the basis functions are centred at the position of the nuclei and therefore moving the nuclei will change integrals over the basis functions. These additional terms are called Pulay forces. They are missing when the Hellmann-Feynman theorem is applied and therefore Hellmann-Feynman forces often differ substantially from energy derivative forces in the case of a local basis set (see [1] and references therein).

Density matrix derivatives are difficult to evaluate. However, for the solution of the Hartree-Fock equations, this problem can be circumvented and instead a new term is introduced, the so-called energy-weighted density matrix which is easily evaluated [12]. However, this is only strictly correct for the exact Hartree-Fock solution. In practice, convergence is achieved up to a certain numerical threshold (e.g. a convergence of $10^{-6} E_h$ of the total energy corresponding to $27.2114 \times 10^{-6} eV$). For very accurate gradient calculations, it may be necessary to make this threshold even lower. The remaining main problem is to generate all the derivatives of the integrals. In a second step, these derivatives have to be mixed with the density matrix.

Evaluation of integrals

In this section we summarise the types of integral which occur.

The simplest type is the overlap integral between two basis functions at two centres:

$$S_{\mu\nu\vec{R}_k\vec{R}_l} = \int \phi_\mu(\vec{r} - \vec{R}_k)\phi_\nu(\vec{r} - \vec{R}_l)d^3r \quad (4)$$

Obviously we can shift \vec{R}_k to the origin, and suppressing $\vec{0}$ in the notation, we obtain:

$$S_{\mu\nu\vec{R}_i} = \int \phi_\mu(\vec{r})\phi_\nu(\vec{r} - \vec{R}_i)d^3r \quad (5)$$

with $\vec{R}_i = \vec{R}_l - \vec{R}_k$.

A kinetic energy integral has the form:

$$T_{\mu\nu\vec{R}_i} = \int \phi_\mu(\vec{r})(-\frac{1}{2}\Delta_{\vec{r}})\phi_\nu(\vec{r} - \vec{R}_i)d^3r \quad (6)$$

the nuclear attraction integral has the form:

$$N_{\mu\nu\vec{R}_i} = \int \phi_\mu(\vec{r})\frac{Z_c}{|\vec{r} - \vec{A}_c|}\phi_\nu(\vec{r} - \vec{R}_i)d^3r \quad (7)$$

and the electron-electron interaction has the form:

$$B_{\mu\nu\vec{R}_i\tau\sigma\vec{R}_j} = \int \frac{\phi_\mu(\vec{r})\phi_\nu(\vec{r} - \vec{R}_i)\phi_\tau(\vec{r}')\phi_\sigma(\vec{r}' - \vec{R}_j)}{|\vec{r} - \vec{r}'|}d^3rd^3r' \quad (8)$$

These integrals are in principle sufficient to deal with molecules. In the case of periodic systems, new types of integrals appear (e. g. multipolar integrals, integrals over the Ewald potential and its derivatives) [11, 13, 14].

The fast evaluation of integrals is one of the main issues in the development of quantum chemistry codes. CRYSTAL uses a McMurchie-Davidson algorithm [15]. Its idea is to map a product of two Gaussian type orbitals at two centres in an expansion of Hermite polynomials at an intermediate centre. This algorithm has proven to efficiently evaluate integrals, although in recent years progress in this specialised field of quantum chemistry has been made (see for example the introduction in [16] or two recent reviews [17, 18]).

The expansion [15, 14] looks like:

$$\phi(\alpha, \vec{r}-\vec{A}, n, l, m)\phi(\beta, \vec{r}-\vec{B}, n', l', m') = \sum_{t,u,v} E(n, l, m, n', l', m', t, u, v)\Lambda(\gamma, \vec{r}-\vec{P}, t, u, v) \quad (9)$$

with $\gamma = \alpha + \beta$ and $\vec{P} = \frac{\alpha\vec{A}+\beta\vec{B}}{\alpha+\beta}$. Λ is a so-called Hermite Gaussian type function

$$\Lambda(\gamma, \vec{r}-\vec{P}, t, u, v) = \left(\frac{\partial}{\partial P_x}\right)^t \left(\frac{\partial}{\partial P_y}\right)^u \left(\frac{\partial}{\partial P_z}\right)^v \exp(-\gamma(\vec{r}-\vec{P})^2) \quad (10)$$

The start value $E(0, 0, 0, 0, 0, 0, 0, 0, 0) = \exp(-\frac{\alpha\beta}{\alpha+\beta}(\vec{B}-\vec{A})^2)$ can be verified by inserting it in equation 9. It can be derived from the Gaussian product rule [19, 20]:

$$\exp(-\alpha(\vec{r}-\vec{A})^2)\exp(-\beta(\vec{r}-\vec{B})^2) = \exp\left(-\frac{\alpha\beta}{\alpha+\beta}(\vec{B}-\vec{A})^2\right)\exp\left(-(\alpha+\beta)\left(\vec{r}-\frac{\alpha\vec{A}+\beta\vec{B}}{\alpha+\beta}\right)^2\right) \quad (11)$$

General values $E(n, l, m, n', l', m', t, u, v)$ are obtained from recursion relations [15, 14]. The E -coefficients depend on the distance $(\vec{B}-\vec{A})$, but not on \vec{P} or \vec{r} . All the integrals can be expressed in terms of E -coefficients [15, 14, 11, 13].

Evaluation of gradients of the integrals

One of the issues of the gradient project is to generalise the algorithms used to generate the energy integrals to obtain the gradients of the integrals. This made a new implementation of recursion relations necessary which are used to obtain the coefficients G in the expansion of the gradients of the integrals in Hermite polynomials.

$$\frac{\partial\Phi(\alpha, \vec{r}-\vec{A}, n, l, m)\Phi(\beta, \vec{r}-\vec{B}, n', l', m')}{\partial A_x} = \sum_{t,u,v} G_x^A(n, l, m, n', l', m', t, u, v)\Lambda(\gamma, \vec{r}-\vec{P}, t, u, v) \quad (12)$$

Once the coefficients are known, the integration can be performed. The integration for the case of gradients of integrals is similar to the case of integrals for the total energy. The only difference is that, instead of the coefficients

$$E(n, l, m, n', l', m', t, u, v)$$

which enter the energy expression, the gradient coefficients

$$G_x^A(n, l, m, n', l', m', t, u, v), G_y^A, G_z^A, G_x^B, G_y^B, \text{ and } G_z^B$$

are used. The coefficients G_x^B can efficiently be obtained together with the coefficients G_x^A [21].

For example, the evaluation of the overlap integral is done as follows:

$$\begin{aligned}
S_{\mu\nu\vec{R}_i} &= \int \phi_\mu(\vec{r})\phi_\nu(\vec{r} - \vec{R}_i)d^3r = \\
&\int \sum_{t,u,v} E(n,l,m,n',l',m',t,u,v)\Lambda(\gamma,\vec{r} - \vec{P},t,u,v)d^3r = \\
&\int E(n,l,m,n',l',m',0,0,0)\Lambda(\gamma,\vec{r} - \vec{P},0,0,0)d^3r = \\
&ME(n,l,m,n',l',m',0,0,0)
\end{aligned}$$

From the first line to the second, we have used the McMurchie-Davidson scheme, from the second to the third we exploited a property of the Hermite Gaussian type functions: all the integrals of the type $\int \Lambda(\gamma,\vec{r} - \vec{P},t,u,v)d^3r$ with $t \neq 0$ or $u \neq 0$ or $v \neq 0$ vanish because of the orthogonality of these functions. The integration (from the third to the fourth line) is trivial. M is a normalisation constant.

Calculating the gradient is easy once we know the new expansion:

$$\begin{aligned}
\frac{\partial S_{\mu\nu\vec{R}_i}}{\partial A_x} &= \frac{\partial}{\partial A_x} \int \phi_\mu(\vec{r})\phi_\nu(\vec{r} - \vec{R}_i)d^3r = \\
&\int \frac{\partial \sum_{t,u,v} E(n,l,m,n',l',m',t,u,v)\Lambda(\gamma,\vec{r} - \vec{P},t,u,v)}{\partial A_x} d^3r = \\
&\int \sum_{t,u,v} G_x^A(n,l,m,n',l',m',t,u,v)\Lambda(\gamma,\vec{r} - \vec{P},t,u,v)d^3r = \\
&\int G_x^A(n,l,m,n',l',m',0,0,0)\Lambda(\gamma,\vec{r} - \vec{P},0,0,0)d^3r = \\
&MG_x^A(n,l,m,n',l',m',0,0,0)
\end{aligned}$$

This way, all the derivatives can be calculated! There are some integrals which involve three centres (for example nuclear attraction) where we exploit translational invariance:

$$\frac{\partial}{\partial C_x} = -\frac{\partial}{\partial A_x} - \frac{\partial}{\partial B_x} \tag{13}$$

because the value of the integral is invariant to a simultaneous uniform translation of the three centres. Four centre integrals can be reduced to a product of two integrals over two centres which makes the calculation of gradients straightforward.

As a whole, the calculation of gradients of the integrals is closely related to calculating the integrals itself. This means that most of the subroutines can be used for

the gradient code. One of the main differences is that array dimensions need to be changed - dealing with gradients is similar to increasing the quantum number (a derivative of an s -function is a p -function, and so on). However, the task of adjusting the subroutines should not be underestimated.

After obtaining the derivatives of the integrals, we mix them with the density matrix just like in the energy calculation. We have to take into account the new term which arose because we did not calculate a density matrix derivative — the energy weighted density matrix. Again, coding this additional term can be done by modifying existing subroutines. After this, we finally obtain the forces on the individual atoms.

Results from test calculations

In this section, we summarise results from test calculations. We have considered the CO molecule which was arranged as a single molecule, as a molecule which is periodically reproduced with a periodicity of 4 Å in one spatial direction ("polymer"), periodically reproduced with a periodicity of 4 Å in two spatial directions ("slab"), and periodically reproduced with a periodicity of 4 Å in three spatial directions ("solid"). Because of the large distance of 4 Å, the molecules can be considered as nearly independent and the forces are quite similar. Still, the calculation of energy and gradient is completely different and therefore this is an important test of Ewald technique and multipolar expansion. The results are given in table 1. The results agree in the best case to at least 6 digits which is the numerical noise and in the worst case up to 4 digits. The difference between analytic and numerical gradients in periodic systems mainly originates from an approximation made within the evaluation of the integrals [22] and from the number of \vec{k} -points which affects the accuracy of the energy-weighted density matrix.

In table 2, we display results from a MgO solid with one oxygen atom slightly distorted from the symmetrical position. Again, the forces agree well up to 5 digits with numerical derivatives.

Future developments and Conclusion

The present version of the code is able to calculate Hartree-Fock forces for periodic systems up to a precision of 4 and more digits. There is no extra disk space needed and the additional memory usage is moderate. This code will certainly be useful for structural optimisation and for future program development towards molecular dynamics or the calculation of response functions. The present version, however, is not yet ready for a release. Instead, the following steps are necessary: Firstly, the usage of symmetry must be implemented. This is of highest importance to make the code fast enough so that it can be used for practical optimisations. We expect

Table 1: Force on a CO molecule with a carbon atom located at (0 Å, 0 Å, 0 Å) and an oxygen atom located at (0.8 Å, 0.5 Å, 0.4 Å). In the periodic case, the molecule is generated with a periodicity of 4 Å. This means, that in one dimension, for example, there would be other molecules with a carbon atom at ($n \times 4$ Å, 0 Å, 0 Å) and an oxygen atom at ($(n \times 4 + 0.8)$ Å, 0.5 Å, 0.4 Å), with n running over all positive and negative integers. Forces are given in $\frac{E_h}{a_0}$, with $E_h = 27.2114$ eV and $a_0 = 0.529177$ Å. Higher ITOLs means a lower level of approximation in the evaluation of the integrals [22].

| Periodicity: | 0D (molecule) | 1D (polymer) (higher ITOLs) | 2D (slab) | 3D (solid) (more \vec{k} -points) |
|------------------|---------------|-----------------------------|-----------|-------------------------------------|
| numerical force | 0.376914 | 0.37660 (0.37664) | 0.37631 | 0.37566 (0.37566) |
| analytical force | 0.376913 | 0.37663 (0.37665) | 0.37633 | 0.37588 (0.37578) |

Table 2: Forces (in $\frac{E_h}{a_0}$) on the atoms of an MgO solid. The MgO solid was chosen to have an artificially high lattice constant of 6.21 Å to make the calculation faster. Coordinates are given in fractional units, e. g. the second Mg is at 0 Å, 0.5×6.21 Å, 0.5×6.21 Å. A normal fcc lattice would be obtained if the sixth atom (Oxygen at 0.53, 0, 0) was at (0.5, 0, 0). Moving this atom from its normal position has led to the nonvanishing forces.

| atom | centred at | analytical force | numerical force |
|------|----------------|------------------|-----------------|
| Mg | (0.0 0.0 0.0) | -0.03018 | -0.03019 |
| Mg | (0.0 0.5 0.5) | -0.00314 | -0.00314 |
| Mg | (0.5 0.0 0.5) | 0.00895 | 0.00895 |
| Mg | (0.5 0.5 0.0) | 0.00895 | 0.00895 |
| O | (0.5 0.5 0.5) | -0.00379 | -0.00379 |
| O | (0.53 0.0 0.0) | 0.00429 | 0.00430 |
| O | (0.0 0.5 0.0) | 0.00746 | 0.00746 |
| O | (0.0 0.0 0.5) | 0.00746 | 0.00746 |

that a version of the present code with symmetry will already be fast enough to compete with numerical derivatives. Further developments will be the coding of the bipolar expansion (a method to evaluate the electron-electron repulsion integrals faster), and sp -shells (s and p shells are often chosen to have the same exponents to make the evaluation of integrals faster). Also, the newly written subroutines are not yet optimal and they will certainly go through a technical optimisation (more efficient coding). In later stages, the code should be made applicable to metals (there is an extra term coming from the shape of the Fermi surface [23] which is not

yet coded) and to magnetic systems (unrestricted Hartree-Fock gradients). Finally, pseudopotential gradients and density functional gradients should be included.

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3 SRRTNet - a new global network

Frascati '99 - Birth of a Network

Scientific Meeting

From the 23rd to the 25th September 1999, a workshop on *Theory and Computation for Synchrotron Radiation* was held at the laboratory in Frascati just outside Rome, Italy. This was the third in an ongoing series of meetings on various aspects of synchrotron radiation, and follows meetings on *Theory and Computation for Synchrotron Applications* held at the Advanced Light Source in Berkeley in October 1997 and *Needs for a Photon Spectroscopy Theory Center* held at the Argonne National Laboratory in August 1998.

This was an excellent meeting, featuring a variety of high quality scientific presentations from both experimental and theoretical participants. The first day was devoted to presentations concentrating on resonant x-ray processes and orbital ordering effects, particularly in V_2O_5 . The second day then moved on to discussions of photoemission, photoelectron diffraction and holography, and studies of high T_c superconductors. This day was concluded with an excellent conference dinner which finished rather late! The final day then concluded with discussions of EXAFS, and x-ray spectroscopies. The overheads used in all the presentations can be viewed on line at <http://wwwsis.lnf.infn.it/talkshow/srrtnet99.htm>

SRRTNet Discussions

The Friday programme also included a two hour session devoted to the idea of forming a global network concentrating on theory for synchrotron radiation research based research. The session began with a talk from Michel Van Hove of the Lawrence Berkeley National Laboratory who outlined the purposes and function of the proposed network. This was then followed by presentations by John Rehr of the University of Washington who highlighted moves to extend the synchrotron radiation research theory network (SRRTNet) in North America, by Maurizio Benfatto of the INFN Frascati, who presented the European perspective, by Kenji Makoshi of Himeji Institute of technology who discussed the Japanese efforts and by Adrian Wander of the Daresbury Laboratory who presented CCP3 as a possible model of how the network could be run. The concept of establishing a global network was received with enthusiasm from all present.

Outcome

Given the support of the meeting for the concept of global network of this sort, it was decided to extend SRRTNet into the global arena. The aims of the network are:

- To provide a central repository for information of relevance to synchrotron radiation research
- To develop theoretical methods pertaining to the experiments performed on synchrotron facilities
- To provide state of the art and user friendly software for the analysis and interpretation of experiments
- To provide training in the use of relevant software through workshops and site visits
- To host visiting scientists
- To hold periodic workshops for the dissemination of new results and methodologies

The directors of the network are Michel Van Hove and John Rehr. As a first step in the development of the network, Daresbury has agreed to host the web pages, and theoretical groups have been contacted and asked to provide input to this central web hub of what will grow into a globe encompassing network. If you are interested in contributing to the network and missed our e-mail announcement, the invitation letter follows;

Dear Colleague,

You may know of the recently established Synchrotron Radiation Research Theory Network (SRRTNet). We are contacting you to invite you, and all theorists interested in this topic, to actively participate in the next phase of the network.

SRRTNet aims to provide theory for experiments that use synchrotron radiation, by means of a global, web-based network linking theoretical and experimental research groups. The driving philosophy is to promote interactions between theory and experiment for mutual benefit, by means of web-based information, workshops, exchange of theoretical methods and computer codes, as well as establishing visiting scientist programs.

At the last SRRTNet workshop, conducted at Frascati near Rome in September 1999, it was decided to strengthen the global character of this network by establishing a central, web-based source of information. Daresbury Laboratory is hosting this web site with Dr. Adrian Wander acting as editor. It is anticipated that all synchrotron facilities will provide direct links for their users to this web site, and consequently we expect this site to grow into an essential resource for synchrotron radiation researchers.

An important first function of the web site will be to provide information about theorists' research interests and links to relevant web pages. The network will be all the more valuable as this coverage becomes complete: it will thus allow theorists and experimentalists alike to find the best sources of information about the various methods for solving specific scientific problems.

The purpose of this message is to ask you to provide such information and links about your group. You may visit the new web site <http://www.cse.clrc.ac.uk/Activity/SRRTNet> and see not only an overview of the network in general, but also the beginnings of such information about specific theoretical groups.

The idea is to put a list of your research topics on the SRRTNet web site, while providing links to your own web site for more detailed and up-to-date information. If you prefer, the SRRTNet site can itself host a more complete web page covering your activities.

The information we wish to present (or link to) includes as many as possible of the following items:

- *your topics of scientific activity related to synchrotron radiation (directly or by methodology);*
- *your computer codes, with their capabilities and availability;*
- *your publications, such as abstracts, papers, databases and web-presentations;*
- *how to contact you or your group.*

Of course, we welcome any links to other information of value to this community. We also welcome receiving the names of other theorists who are not yet on our mailing list, so feel free to forward this message to them as well.

Please send all information for posting on the SRRTNet web site to srrtnet@dl.ac.uk (c/o Dr. Adrian Wander). Should you need more motivation to provide the above information, please consider that:

- *the SRRTNet web site complements normal publications and conference presentations, by globally exposing your work round-the-clock to a targeted audience, as soon as you deem it publishable;*
- *your participation in the network will help define topics for workshops that bring together theory and experiment;*
- *the required effort on your part is very modest, and minimal if you already have a web site that describes your work.*

We look forward to your participation in SRRTNet, thereby making it a most valuable research tool for the scientific community.

Michel Van Hove and Adrian Wander

As the network grows, it is envisaged that the web site will grow to include details of experimental groups working with synchrotron radiation as well. The network will then become an invaluable tool for everyone working in the field.

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4 High performance computing

4.1 Cluster-Computing Developments in the UK

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Introduction

A "cluster" is a collection of complete computers (nodes) that are physically interconnected by a high-performance "local area network" (LAN). Typically each node is a workstation or personal computer (PC). Clusters permit running parallel jobs using PVM or MPI implemented over the network as well as permitting independent use of the nodes for task farming.

The advantages of cluster computing derive from the fact that off-the-shelf commodity components are used. This offers a cost-effective solution to medium-scale computing requirements.

For a good introduction to the concepts of cluster computing and architectures available see "Scalable Parallel Computing" by K. Hwang and Z. Xu (WCB/McGraw-Hill, 1998, ISBN 0-07-031798-4).

Cluster computing solutions in the USA are becoming mainstream and may become the dominant system of the future for computational science. A 64x2-way Alpha-based system built by Alta Technology and installed at the University of New Mexico has been accepted into the USA Alliance computational meta-computing grid. A similar system, the CPlant, see <http://www.cs.sandia.gov/cplant>, is supported by Compaq under a 4-year agreement with the US DoE and is now being used at Sandia National Laboratory with a Myrinet high-performance switch for enhanced communications. This system forms part of the Accelerated Strategic Computing Initiative (ASCI) Path Forward programme.

One of the first projects, the Beowulf, was started at NASA in 1994, see <http://www.beowulf.org>. This Web page also contains links to many related sites worldwide. Commodity cluster systems are now often known as Beowulf-class computers.

It is important for UK scientists to be able to evaluate this kind of equipment for parallel computing, as has been noted by EPSRC in recent surveys. Daresbury Laboratory therefore, as part of the Distributed Computing (DisCo) Programme, has built a 32-processor Beowulf cluster using 450 MHz Pentium III processors. Currently the processors, which are in the form of off-the-shelf PCs, each with

memory and disk but no keyboard or monitor, are connected by dual fast Ethernet switches – 2x Extreme Summit48, one network for IP traffic (e.g. nfs) and the other for MPI message passing. Additional 8-port KVM switches are used to attach a keyboard and monitor to any one of the nodes for administrative purposes. The whole cluster has a single master node (with a backup spare) for compilation and resource management. All nodes are currently running RedHat Linux v6.0.

Applications, such as GAMESS-UK, DL_POLY, ANGUS, CRYSTAL, POLYMERSEM, REALC and CASTEP are being ported to the system for evaluation. Results showing their performance will be posted on the DisCo Web site as they become available, see

<http://www.cse.clrc.ac.uk/Activity/DisCo>.

Over the coming months we also plan to evaluate a variety of networking and software options for the system. Some of the options are summarised below. Prices vary, as does performance and robustness, and it is not yet clear what will be the preferred solution for building a large-scale compute server.

Network Options

| network | latency (μ s) | bandwidth (MB/s) |
|--------------------|--------------------|------------------|
| fast Ethernet | 50 | 12.5 |
| Gigabit Ethernet † | 9.6 | 93 |
| Myrinet | 20 | 62 |
| QSW QsNet ‡ | 5 | 210 |

† Gamma project with Packet Engines NIC.

‡ MPI short message protocol.

Figures in the table are subject to confirmation and depend on what driver hardware and software is used.

Message-passing Options

Message passing options include implementations of MPI and PVM, but there are others too.

MPICH – Argonne National Laboratory’s implementation of MPI

<http://www-unix.mcs.anl.gov/mpi/mpich/index.html>

LAM/MPI – Local Area Multicomputer MPI, developed at the Ohio Supercomputer Center and Univ. of Notre Dame <http://www.mpi.nd.edu/lam>

Globus – Metacomputing Environment <http://www.globus.org/>

Compilers

Widely-used compilers include the Gnu family, Portland Group, KAI, Fujitsu, Absoft, NAG etc.. Compaq has released AlphaLinux compilers which are reputedly excellent. Some people already compile their applications under Digital Unix and run them on Alpha Linux, although this is not permitted under the license conditions.

Absoft Corp. – FORTRAN77 (f77) and Fortran 90 (f90) <http://www.absoft.com>

The Portland Group (PGI) – High Performance Fortran (pghpf), FORTRAN77 (pgf77), C and C++ (pgcc) <http://www.pgroup.com>

Numerical Algorithms Group (NAG) – FORTRAN 90 (f90), Fortran 95 (f95) <http://www.nag.com>

Gnu C – free FORTRAN77, C, Pascal, and C++ compilers <http://gcc.gnu.org/>

BERT 77 – described as "an automatic and efficient Fortran paralleliser" <http://www.plogic.com/bert.html>

Lahey/Fujitsu – LF95 Linux Express fully optimising Fortran 95 compiler <http://www.lahey.com>

Compaq - Fortran for Linux Alpha (free under certain conditions to academics) <http://www.compaq.com/fortran/>

Compaq - C for Linux Alpha http://www.unix.digital.com/linux/compaq_c/index.html

Numerical Libraries

ASCI Option Red software – BLAS, fast-Fourier transform, hardware performance-monitoring utilities, extended-precision and maths primitives are all available free under restricted licenses

<http://www.cs.utk.edu/~ghenry/distrib/archive.htm>

NAG Parallel Library – a version tuned for Beowulf systems is available commercially <http://www.nag.co.uk>

Resource Management and Job Scheduling Options

LSF – Load Sharing Facility from Platform Computing <http://www.platform.com>

LobosQ – queuing system from NIH, Bethesda USA <http://www.lobos.nih.gov>

PBS – Portable Batch System developed at NASA Ames Research Center now commercially available from MRJ Inc. <http://pbs.mrj.com>

Virtual Private Server – new software infrastructure for scalable internet services and enterprise services from Sychron Ltd. Oxford. <http://www.sychron.com>

DQS – Distributed Queueing System. A free batch queueing system
<http://www.scri.fsu.edu/~pasko/dqs.html>

BVIEW – monitoring software
<http://w272.gsfc.nasa.gov/~udaya/Public/software/bview/bview.html>

bWatch – monitoring software <http://www.sci.usq.edu.au/staff/jacek/bWatch>

BPROC – making processes visible across nodes, allowing fork()s to happen across nodes, allowing process migration, allowing kill()s to work across nodes, currently pre-alpha release <http://www.beowulf.org/software/bproc.html>

Cluster patches for procps – lets you compile /proc-based programs like ps so they report on all processes on the cluster, not just the ones on the machine you're logged into <http://www.sc.cs.tu-bs.de/pare/results/procps.html>

SMILE Cluster Management System – Run commands on all nodes, shut down individual nodes and sets of nodes, monitor health of nodes. Makes clusters easier to administer. <http://smile.cpe.ku.ac.th/software/scms/index.html>

Parallel Virtual Filesystem – LD_PRELOAD-based filesystem modification to let you transparently stripe big files across many disks. Allows high-performance access to big datasets. <http://ece.clemson.edu/parl/pvfs>

Scripts for configuring 'clone' worker nodes – makes adding nodes to a Beowulf painless
<ftp://ftp.sci.usq.edu.au/pub/jacek/beowulf-utils/disk-less>

Scripts for doing various things on a cluster, backups, shutdowns, reboots, running a command on every node
ftp://ftp.sci.usq.edu.au/pub/jacek/beowulf-utils/misc_scripts

Software is being added to the public domain on a daily basis, see for instance "The Beowulf Underground" URL <http://www.beowulf-underground.org>

Other Beowulf Clusters in the UK

There are a number of other Beowulf systems being built in the UK. We list just a few of them on the DisCo Web page at URL <http://www.cse.clrc.ac.uk/Activity/DisCo>. These include: Enterprise and Voyager (Cambridge), The Borg (Cranfield), University of Glasgow, Stac Follaidh (Lancaster), HPCI (Southampton), MadDog (UMIST).

Some Commercially available Systems

WorkstationsUK – <http://www.workstationsuk.demon.co.uk>

InSiliCo – <http://www.insilico.co.uk>

SALT – Commercial Hardware Vendor in Germany <http://www.suse.de>

Sybrandt Open Systems – provides a commercial Beowulf solution
<http://www.sybrandt.com>

Paralline – distributes Linux clusters, high-speed networks and services
<http://www.paralline.com>

ParTec – supports the ParaStation project and sells clusters and services
<http://www.par-tec.com>

See also the NASA Web site mentioned above.

An Example

As an example of our initial experiences using the Daresbury Beowulf we show the performance from the CRYSTAL98 electronic structure code in small RHF calculations on the Chabazite and TiO_2 structures. Results from the 450 MHz Pentium III system are compared with the Cray T3E-1200E. Clearly the single-node performance of the Pentium III is good compared to the 600 MHz DEC Alpha EV5 in the Cray, but the latter offers superior scalability for parallel programs needing a large number of processors. We note that in these small test cases there was some poor load balancing for the 16 and 32 processor runs.

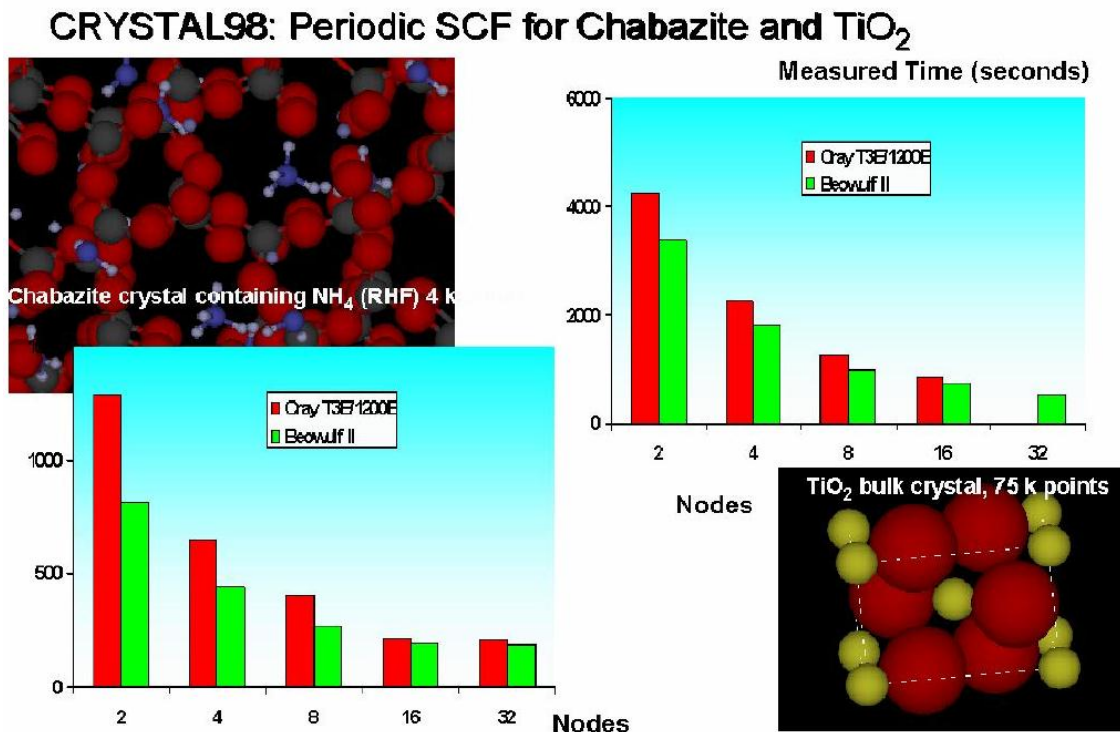


Figure 1: CRYSTAL 98 benchmarks

4.2 New HPC Support Mechanisms

Daresbury Laboratory and University of Edinburgh are collaborating with University of Manchester to provide future HPC support.

Future Mechanisms for HPC Support from EPSRC

The current funding for the three UK HPCI Centres ended at the end of October 1999. The future HPC support mechanisms which were approved by EPSRC's High Performance Computing Strategy Committee (HSC) in June 1999 are now in place following the response to calls for proposals from centres for both Dedicated Consortium Support and Core Activities.

The Dedicated Support funding from EPSRC now contains two strands:

- Ongoing Dedicated Support for research groups and HPCI Consortia with existing grants at the Daresbury and EPCC HPCI Centres until the end of that grant;
- Dedicated Support for individual research groups applying for new grants either within the research group or at a high-end computing centre (e.g. Daresbury, EPCC or CSAR) of the research group's choice. This will be peer-reviewed via the normal programme lines.

Support for the existing scientific consortia is continuing at Daresbury and EPCC until their current research grants end. In addition to this consortia previously mapped to Southampton have been re-assigned to either Daresbury or EPCC as follows:

- o Daresbury: Materials Chemistry (Prof. Catlow, RI), DNS of Fluids (Prof. Sandham, Southampton), Liquid Crystals (Prof. Allen, Bristol)
- o EPCC: UGAMP (Prof. O'Neill, Reading), OCCAM (Dr. Webb, Southampton), Geophysics (Prof. Price, Birkbeck)

Future requests to EPSRC for Dedicated Support for individual research groups should be made to the appropriate Research Council. Other Research Councils are currently making their own arrangements.

Core Support Activity

EPSRC provided separate funding, via a call for proposals, for a Core Activity to track and disseminate information on developing standards in software and tools

and to promote good programming practice. This is to be provided by the "UK-HEC Collaboration", a collaboration between Daresbury, EPCC and the Manchester Research Centre for Computational Science (MRCCS).

The UK-HEC Collaboration will investigate underlying HPC issues relating to hardware and software technology which might enhance the effective use of HPC resources in the UK. This includes programming languages (e.g. C, Java, Fortran95), software engineering and QA, data management, visualisation and VR, and meta-computing. Technical reports will be produced and short courses and workshops held in key areas. Information will be announced via HPCProfile and the Web pages (see below).

New HPCI Web pages

EPCC and Daresbury Laboratory are collaborating to provide new Web pages with appropriate URL for their diverse HPC activities. Links to all the supported consortia and related activities will be provided via these pages which will complement those at CSAR. The draft pages can be found at <http://www.cse.clrc.ac.uk/ListActivities/CLASS=5;CLASSTYPE=43;> . Please note that the URL will be simplified shortly. We have applied to UKERNA for DNS addresses www.hpci.ac.uk and www.uk-hec.ac.uk . We invite your comments on the kind of material you would like to see here.

HPCProfile

The last issue of HPCProfile in its current form appeared in December 1999. As a part of the UK-HEC collaboration we shall be producing two issues a year starting in 2000 devoted to HPC programming techniques and underlying computing issues. This will be supplemented by other material which will provide information on the Dedicated Consortium Support, CCPs and Distributed Computing Programme (DisCo).

Further Information

In addition to looking at the existing Web pages you can contact:

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<http://www.csar.cfs.ac.uk>

5 Reports on visits

Over the past six months CCP3 has provided support for a number of visiting scientists. Reports on these visits follow

Prof. Lars Hedin

Lars Hedin, Emeritus Professor of Theoretical Physics at the University of Lund, Sweden, visited the physics departments in Cardiff and York, from 28 June to 7 July 1999. This visit was supported by CCP3 as part of the guest scientist programme. In both departments he gave a seminar on one of his current research interests, "The transition from the adiabatic to the sudden limit in core level photoemission". John Inglesfield (Cardiff) has worked with Lars Hedin on this topic, and the visit has facilitated future collaboration. In York, Professor Hedin provided many helpful comments during discussions with Rex Godby and his group on topics of joint interest concerning self-energy calculations and total energy from many-body perturbation theory, and with Jim Matthew and members of his group concerning electron spectroscopy.

Rex Godby (University of York) and John Inglesfield (University of Wales Cardiff)

Dr HM Tütüncü

Dr Tütüncü visited GP Srivastava at the University of Exeter

Dr Tütüncü investigated the phonon dynamics of the Si(001)/Bi(2x1) surface by employing the adiabatic bond charge model. The atomic geometry and electronic charge density corresponding to the Bi-Bi dimer was obtained from *ab initio* pseudopotential calculations.

Two characteristic peaks in the phonon density of states were found to develop upon the adsorption of the Bi monolayer. One of these lies in the optical region of the bulk Si phonon density of states. The other peak lies below the Si bulk acoustic peak, and results from the Rayleigh modes corresponding to the heavier Bi atoms. It is suggested that the latter feature could be detected in helium atom scattering or high resolution electron loss experiments. The work was presented in September 1999 at the ECOSS18 in Vienna.

We appreciate the financial support provided by CCP3.

GP Srivastava
University of Exeter

Dr M Çakmak

Dr Çakmak also visited GP Srivastava at the University of Exeter.

Dr Çakmak performed *ab initio* pseudopotential calculations of atomic and electronic structures of semiconductor surfaces covered by small molecules. In particular he made some progress towards understanding dissociative adsorption of Si_2H_6 on $\text{Si}(001)$. We hope to provide an analysis of these results in the future.

We would like to thank CCP3 for financial support.

GP Srivastava
University of Exeter

Prof. David Vanderbilt

Prof. Vanderbilt visited Daresbury Laboratory and the Faraday Discussion 114 meeting in Ambleside. A report on his visit to Daresbury follows:

Prof. Vanderbilt's visit supports the CASTEP Linear-Response Theory Project

Professor David Vanderbilt visited us in August as part of a collaboration on density-functional perturbation theory (DFPT). Prof. Vanderbilt was the creator of ultrasoft pseudopotentials (USP's) which dramatically increase the efficiency of plane-wave DFT calculations. We are drawing on this expertise to extend the linear-response formalism to include USP's. At the abstract (operator) level this has been achieved, paving the way for the development of the implementation details and coding within the CASTEP program.

The combination of linear-response theory (LRT) with density-functional methods has a strong appeal. Everyone knows how successful DFT has been when applied to condensed-matter problems, how quickly the simulator's horizons are expanding, and how exciting the future looks. However, escaping from the "zero-K, ground-state plane" remains a major challenge: how are we to tackle the calculation of time-dependent or statistical-mechanical quantities? What about vibrational spectra, or excited states? In these matters molecular dynamics is sure to be a leading technology, but methods based on a perturbative approach have a separate key role to play. Linear-response theory predicts the response of condensed-matter systems to perturbations. The link to DFT comes when the perturbations are phrased as changes in the external potential. The perturbation may be due to ionic motion, elastic strain, electric and magnetic fields and even "alchemical" changes to atomic identity. Some of the properties that may be calculated are phonon spectra, elastic constants, Born effective charges, dielectric tensors and chemical shifts.

Independent research by Karin Rabe (Yale) and Xavier Gonze (then at Corning) laid the foundations for the variational calculation of the response of a system described by a DFT Hamiltonian to a perturbation. A variational expression equates the second-order change in the total energy to the minimum of a functional expression in the first-order changes of the one-electron wavefunctions, and minimisation of this expression (using e.g. conjugate gradients) yields the diagonal part of the second-order energy. Cross-derivatives may be found from non-stationary expressions in the first-order wavefunctions, or alternatively from stationary expressions involving two simultaneous perturbations. Other methods extract the same information by different means, notably that pioneered by Baroni *et al*, where schemes analogous to the self-consistent solution of the Schrödinger equation are used. Both these approaches have the great advantage that the perturbation need not be commensurate with the simulation cell, as it must be in frozen phonon and similar calculations.

One of my projects is to implement linear-response calculations in the CASTEP plane-wave code, a natural home for DFPT calculations. Both Karin and Xavier developed DFPT in plane-wave codes which used separable non-local pseudopotentials. A plane-wave basis is a strong advantage, since derivatives are easily calculated. This is important because the change with respect to the perturbation in the potential can be formulated using derivatives of the plane waves. Even given the simplicity of a plane-wave basis, the DFPT formalism is involved and its implementation a large task. Moreover, a sizeable piece of the jigsaw was missing until recently, because the extra complications introduced by Vanderbilt ultrasoft pseudopotentials (USP's) had not been addressed. Nowadays, USP's are a must in plane-wave calculations, and we therefore needed to extend the DFPT formalism.

It's good to go straight to the top, so who better to ask about USP's than Prof. Vanderbilt himself. Both he and Karin Rabe are consultants to the CASTEP linear-response project, which is a joint venture between Daresbury, the United-Kingdom Car-Parrinello Consortium (UKCP) and Molecular Simulations Inc. (MSI). Prof. Vanderbilt has mapped out the formalism for DFPT-USP calculations in a new, unified scheme. In doing so he has also brought considerable clarity to what was already in the literature by taming the heavy and conflicting notations used by various authors.

The CASTEP LRT project is moving forward on two fronts. Karin Rabe has provided a base code developed on a '92 version of CASTEP. Although much water has passed under the bridge, this is still a most helpful starting point for coding DFPT within modern CASTEP. With this development one will be able to use CASTEP to compute the dynamical matrix, Born effective charges and the static dielectric tensor, albeit with norm-conserving pseudopotentials and within the LDA. In parallel I am developing the USP implementation based on Prof. Vanderbilt's formalism. Once this is complete and in CASTEP it will mark a great stride forward in the code's capability and is sure to spark many exciting applications. Looking even further ahead, there is the possibility of adding other classes of perturbation to further extend the range or properties accessible.

Meeting face-to-face with Prof. Vanderbilt was particularly valuable because of the complexity of this work, and excellent progress was made during his visit to Daresbury. It helped to strengthen our collaboration and enabled a most enjoyable exchange of science and culture, and we thank CCP3 for its support.

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6 Meetings, Workshops, Conferences

6.1 Reports on Bursaries

CCP3 awarded two bursaries to assist students in attending the ECOSS-18 meeting in Vienna. Reports from Yu Chen of the University of Birmingham and Ally Chan of the University of Nottingham on this conference have been received.

Yu Chen reports:

The 18th European Conference on Surface Science (ECOSS-18) was held in Vienna, Austria from September 21-24, 1999. There were around 800 people from all over the world attending this conference.

More than 700 papers were presented in both oral and poster sections during the four days of the conference, which covered a wide range of scientific areas from traditional surface science to new and emerging research areas. As the highlight of the conference, four distinguished scientists were invited to give the plenary lectures. They were: Professor Jürgen Kirschner (Surface Science approach to mesoscopic magnets: Dots, wires, and platelets), Professor Wolf-Dieter Schneider (Nanoscale surface physics: electron confinement, Kondo effect and self-assembly phenomena), Professor Hans-Joachim Freund (Deposited metal aggregates: models for heterogeneous catalysis) and Professor Miquel Salmeron (Energy dissipation processes in friction).

The ECOSS-prize is an award for the best student paper presented at the conference. This year 6 papers were chosen as candidates to compete for this prize. The final decision was made by a committee based on oral presentations at the conference and was announced during a conference dinner. Mr. Krishna Swamy from the University of Innsbruck, Austria, won this year's ECOSS prize.

Thanks are due to CCP3 for their contribution to my expenses attending this conference. I had the opportunity to experience a stimulating and productive meeting. I made an oral presentation on an HREELS study of passivated gold clusters on surfaces, and the discussion afterwards was interesting and encouraging.

ECOSS-19 will take place in Spain next year.

Ally Chan's Report:

This year's European Conference on Surface Science (ECOSS-18) was held at the Vienna University of Technology under the auspices of the Austrian Vacuum Society (ÖGV) and the Surface Divisions of the European Physical Society (EPS) and the International Union for Vacuum Science, Technique and Applications (IUVSTA). The scientific programme comprised a comfortable 4 parallel oral sessions and 3 poster sessions, the highlights of which were the plenary lectures by invited speakers from both European and American institutions. I particularly enjoyed the plenary lecture given by H.-J. Freund (Fritz-Haber Intitut, Germany), on alumina-supported transition metal aggregates as a model for heterogeneous catalysis. Size dependant reactivity studies of the metal clusters towards the adsorption of small molecules, e.g. the thermal dissociation of CO and the photodissociation of CH₄, were discussed. Miguel Salmeron (Lawrence Berkeley National Laboratory, USA) gave an informative and visually entertaining lecture, which elucidated the use of surface imaging techniques (STM and AFM), in conjunction with surface spectroscopies, to probe the mechanisms for energy dissipation at interfaces.

As expected, the contributed papers covered a broad spectrum of topics in Surface Science; however, there was a noticeable emphasis on the more fundamental aspects of surface physics (e.g. electronic properties, structure, diffusion and growth). Contributions on surface chemistry, reactivity and catalysis were somewhat reduced and there were hardly any contributions on surface dynamics. Studies using optical methods (Second Harmonic Generation and Sum Frequency Generation), which was all the rage at last year's International Symposium of the American Vacuum Society (AVS) in Baltimore, had a minimal presence at this conference. Surface microscopy seems increasingly popular, with STM superseding LEED and synchrotron-based X-ray techniques in surface structural investigations. There was a surprisingly limited amount of theoretical work presented and in that, only a handful were on calculations using DFT methods. Personally, I was delighted at the relatively large volume of papers on self-assembled monolayers, though a little disappointed by lack of papers on molecular semiconductor films and on the Surface Science of biological systems.

The poster I presented was on 'The Surface Structure of CF₃ Co-adsorbed with Iodine on Cu(111) by Normal Incidence X-ray Standing Wave (NIXSW) Analysis'. This work is part of a larger project to investigate the degree of rotational freedom exhibited by adsorbed molecules with three-fold symmetry, and the effect of surface coverage and coadsorbates in locking the rotation. In this paper, the ability of the NIXSW technique to accurately track subtle structural changes in both the I and CF₃ fragments as a function of surface coverage was highlighted: in this case, as coverage increases, the I moves in towards the surface while the CF₃ moves outwards from the surface, with the fragment exhibiting a greater degree of rotational freedom. Dr Rob Jones (University of Nottingham, UK) gave a closely related talk on a variation of the NIXSW technique chemical shift XSW as applied to the structural

location of molecular coadsorbates on metal surfaces.

A feature that caught my eye was the thoughtful arrangement of the exhibition of companies, such that individual exhibition booths were positioned in a number of sites near the posters and lecture halls, affording greater visibility to each exhibitor. This appeared to be a superior arrangement to that of a single dedicated exhibition area. For a European conference, there was fair representation from American and Japanese scientists, though the largest representation was by far German, to the point that the conference occasionally had the air of a German Physical Society meeting.

A final note on the conference: Vienna was a superb choice of location, with tremendously enjoyable social facilities within a comfortable walking distance of the conference centre. The scientific programme was good and the continued innovation of the European Surface Science community was apparent in the introduction of several new sessions e.g. ‘nanoparticles & nanowires’ and ‘thin organic layers’. The conference was not too large to preclude easy interaction with other participants. Finally, my personal thanks go to CCP3 for a travel bursary towards this conference.

Ms Ally S Y Chan
School of Chemistry
University of Nottingham
Nottingham NG7 2RD, UK

6.2 Reports from Meetings

Optical Probes at Surfaces

Surface Science Research Centre, Liverpool
29th June 1999

A one day meeting on Optical Probes at Surfaces was held in the Liverpool Surface Science Research Centre on 29th June 1999, sponsored by CCP3. The meeting was attended by 30 scientists from a number of UK laboratories specialising in optical probe applications to surfaces – currently a very active field of research. Invited lectures were given by Prof. M .E. Pemble (Salford), Dr T. Farrell (Liverpool), Dr C. Matthai (Cardiff), Dr A.Taylor (Imperial College) and Prof R. Del Sole (Rome Tor Vergata). Prof. Del Sole was also sponsored by CCP3 to visit Cardiff and York Universities for discussions on surface optical properties.

P. Weightman
Surface Science Research Centre, University of Liverpool

Faraday Discussion 114

The Surface Science of Metal Oxides

St Martin's College, Ambleside, UK
1-3 September 1999

The aim of this discussion was to bring together experimentalists and theoreticians in the field with the aim of defining the state-of-the-art and assessing the prospects for the next few years. The majority view was that these aims were fulfilled

There were 128 participants, with about 50% from the UK, the remainder coming from continental Europe, Israel, North America and Japan. The Invited Lecturer was Prof. Dr. H.-J. Freund from the Fritz-Haber-Institut, who elegantly reviewed the field. It was notable that he had made a point of including work from most of the invited speakers. The Introduction was followed by 24 excellent oral papers. Finally, the summarising remarks were presented in typically professional style by Prof T. E. Madey from Rutgers University.

The amount and depth of the discussion were rather impressive. It was clear that this was the appropriate time to air a number of issues which had become pivotal over the past few years as this area burgeons. This was helped immeasurably by the almost equal number of experimentalists and theoreticians, who often had experimental data and calculations to compare. The electronic structure, crystallography and reactivity of titanium dioxide surfaces played a central although not dominating role in the discussion, arising from its role as a model system. Fifty posters were displayed on the first evening, in what was a very lively and enjoyable session. The

quality of presentations was extremely high, giving the judges for the poster prize a difficult time. As for the weather, it did not rain, although you could not see the top of Wansfell until 5pm on the last day. A fortunate group of 20 stayed around to continue the discussion whilst enjoying a glorious Lake District weekend.

G. Thornton

IRC in Surface Science and Chemistry Department, University of Manchester

6.3 Upcoming meetings

Here is an incomplete list of upcoming meetings which might be of interest for surface scientists. For the latest news, see at the CCP3 webpages. To advertise your conference on the web, please send email to ccp3@dl.ac.uk .

- CMMP 99 IOP Condensed Matter Physics Meeting
University of Leicester, UK 19th-22nd December 1999
<http://conferences@iop.org>
- 18th General Conference of the Condensed Matter Division of the European Physical Society
Montreux, 13th-17th March, 2000
<http://www.eps-cmd18.ch>
- ACS Division of Colloid and Surface Chemistry
Meeting on Semiconductor Surface Chemistry
San Francisco, California, USA, 26th-31st March 2000
<http://www.acs.org/meetings/sanfran2000/>
- 2nd San Luis Symposium on Surfaces, Interfaces and Catalysis
Mar del Plate, Argentina, 3rd-6th April 2000
<http://surface.chem.uwm.edu/conferences.html>
- Summer School on Surface, Interfaces and Catalysis
Mar del Plate, Argentina, 7rd-8th April 2000
<http://surface.chem.uwm.edu/conferences.html>
- International Conference on Thin Film Physics and Applications
Shanghai, China, 8th-11th May 2000
http://physicsweb.org/events/describeconf.phtml?entry_id=658
- JVC-8
8th Joint Vacuum Conference of Croatia, Hungary and Slovenia
Pula, Croatia, 4th-9th June 2000
- 22nd Annual Symposium on Applied Surface Analysis
University Park, Pennsylvania, USA, 7th-9th June 2000
<http://www.outreach.psu.edu/C&I/SurfaceAnalysis2000/>
- 28th IUVESTA Workshop Ion Beam Techniques for the Analysis of Composition and Structure With Atomic Layer Resolution
Sponsored by IUVESTA (International Society for Vacuum Science, Techniques and Applications) and CLRC Daresbury Laboratory
Cosenor's House, Abingdon, Oxfordshire, UK, 26th-30th June 2000

- QSA-11 International Millennium Conf. on Quantitative Surface Analysis
Guildford, UK, 4th-7th July 2000
<http://www.surrey.ac.uk/MME/QSA/>
- International Conference on Solid Films and Surfaces (ICSFS-10)
Princeton University, USA 10th-14th July 2000
<http://www.pmi.princeton.edu/ICSFS/>
- 10th International IACIS Conference on Surface and Colloid Science
University of Bristol, Bristol, UK, 23rd-29th July 2000
<http://www.tlchm.bris.ac.uk/IACIS/IACIShome.htm>
- Many-Particle Spectroscopy of Atoms, Molecules and Surfaces
Halle/Saale, Germany, 26th-29th July 2000
<http://www.mpi-halle.mpg.de/~e2e/mps2000.html>
- Eighth International Conference on Electronic Spectroscopy and Structure
Berkeley, California, USA, 8th-12th August 2000
<http://www-als.lbl.gov/icess/>
- Workshop on Applications of Synchrotron Light to Magnetic Materials
Laboratório Nacional de Luz Síncrotron (LNLS) Campinas, Brazil, 14th-16th
August 2000
<http://www.ifi.unicamp.br/~waslmm/>
- PSI-K2000: Ab initio (from Electronic Structure) Calculations of Complex
Processes in Materials
Schwäbisch Gmünd, 22nd-26th August, 2000
<http://www.dl.ac.uk/TCSC/HCM/PSIK/psi-k2000.html>
- Faraday Discussions 117-Excited States at Surfaces
University of Nottingham, UK, 4th-6th September, 2000
<http://www.rsc.org/lap/confs/faradischeme.htm>
- 9th European Conference on Applications of Surface and Interface Analysis
Marseilles, France, 1st-5th October 2001
<http://www.enscp.jussieu.fr/ECASIA/>



The Second San Luis Symposium on Surfaces, Interfaces and Catalysis

Third Announcement and Call for Papers This is a third announcement and Call for Abstracts for the Second San Luis Conference to be held in Mar del Plata, Argentina from April 3-6, 2000 followed by a Summer School on April 7 and 8, 2000. Abstracts of up to 300 words are requested from those who wish to make either oral or poster presentations. These should to be submitted electronically using the form found at:

<http://surface.chem.uwm.edu/conferences.html>

Background information on the conference, registration information and fees, contact information and links to the city of Mar del Plata can also be found at this web site.

The conference will be followed by a Summer School and students wishing to apply for a fellowship to attend the San Luis Conference and Summer School as well as those wishing to register for the Summer School can do so on the above Web site.

Summer School Topics:

Andy Gellman: Substituent Effects and their Applications to Surface Reactions and Probing of Transition States

Wayne Goodman: Metal Clusters on Planar Oxide Supports

Brian Hayden: Reaction Dynamics on Stepped and Alloy Surfaces

Claude R. Henry: Growth and Morphology of Metal Clusters Supported on Oxide Surfaces

Richard Lambert: Controlling the Performance of Heterogeneous Catalysts: The Use of Alloy Catalysts and Electrochemical Promotion.

William Millman: Support for Catalysis-related Research in the United States: Relation to the Physical and Chemical Sciences and New Directions

Claudine Noguera: Electronic Structure of Oxide Surfaces and Clusters: Modification of the Iono-covalent Character and Screening Effects.

Jose Rodriguez: The use of Synchrotron-based Techniques (Photoemission, XANES and Time-resolved X-ray Diffraction) in Surface Science and Catalysis

William Steele: The Computer Simulation of Molecular Adsorption on Realistic Model Solids

Patricia Thiel: Quasicrystal: A Surface That's Hard to Scratch

Wilfred Tysoe: Synthesis of Model Catalysts from Metal Carbonyls on Alumina

Francisco Zaera: Kinetic Measurements, RAIRS, and Hydrocarbon Chemistry

7 Abstracts of forthcoming papers

In the following is a list of abstracts of forthcoming publications, ordered in the way they were received. Everybody is invited to send abstracts to ccp3@dl.ac.uk.

Medium-Energy Ion Scattering Studies of Two Dimensional Rare-Earth Silicides

D. J. Spence¹, S. P. Tear¹, T. C. Q. Noakes², P. Bailey²

¹Department of Physics, University of York, York, UK YO10 5DD

²CLRC Daresbury Laboratory, Daresbury, Warrington, UK WA4 4AD

Medium-energy ion scattering (MEIS) has been used to determine the atomic structure of 2D rare-earth silicides on Si(111). In the case of Si(111)1x1-Er 2D silicide surface the MEIS results refine previously published results but in the case of the Si(111)1x1-Ho surfaces, this work represents the first full quantitative structural analysis which, for the first time, reveals a structure similar to that of the Si(111)1x1-Er surface and directly supports a model in which a rare-earth monolayer resides below a Si bi-layer close to bulk termination.

Accepted for publication in Phys. Rev. B

Controlling The Lifetime Of Adsorbate Negative Ion States

P. J. Rous

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University of Birmingham, Edgbaston, Birmingham, B15 2TT

We demonstrate theoretically that the lifetime of molecular or atomic negative ions can be controlled by adsorption onto a metallic thin film, a phenomenon that is analogous to the electromagnetic enhancement/inhibition of the lifetime of electronically excited atomic states which decay by spontaneous photon emission. Specifically, we show that by coupling the $^2\Pi_g$ negative ion state of adsorbed N_2 to the quantum well states of a thin film of Ag(111) supported on a Pd(111) the ionic lifetime can be significantly increased or decreased by changing the thickness of the thin film.

Phys. Rev. Lett. (in press)

The Surface Resistivity Of Stepped Al Surfaces

P. J. Rous

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University of Birmingham, Edgbaston, Birmingham, B15 2TT

When an electrical current flows parallel to a stepped metal surface, the steps contribute to the surface-induced resistivity due to the diffuse scattering of the carriers that occurs at the step edges.

In this paper, multiple scattering theory is used to compute the surface resistivity induced by steps on the vicinal (100) surfaces of Al. The carrier scattering by the surface barrier is described by a model corrugated potential fit to a result of a first-principles calculation of the surface-induced resistivity of the unstepped surface. The Bloch states of the semi-infinite bulk are described by a layer-KKR calculation. The surface resistivity is found to be a function of the step density, η_s , and becomes a linear function of η_s for low step-edge densities. Deviation for linearity at higher step densities results from the multiple scattering of carriers between step edges.

Phys. Rev. B (in press)

Nordheim Dependence In The Surface Resistivity Of Disordered Overlayers

P. J. Rous

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A CPA layer-KKR calculation is used to compute the surface resistivity of Cu(100), Al(100) and Al(111) surfaces as a function of coverage by a disordered overlayer of Cu and Al adatoms. The Bloch states of the semi-infinite bulk are described by a layer-KKR calculation combined with the coherent potential approximation to represent the carrier scattering by the disordered overlayer. The diffusion of carriers by the surface disorder results in a Nordheim, or quasi-parabolic, dependence of the induced surface resistivity upon the coverage. This result confirms the qualitative behavior observed in a prior ATA calculation where the surface was modeled as a random distribution of s-wave scatterers in front of a hard-wall potential representing the surface barrier (D.L. Lessie and E.R. Crosson, J. Appl. Phys. **59** 504 (1986)).

Journal of Applied Physics (in press)

Chlorine adsorption on the Cu(111) surface

K. Doll¹ and N. M. Harrison^{1,2}

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² Department of Chemistry, Imperial College, London, SW7 2AY, UK

We investigate the adsorption of chlorine on the Cu(111) surface with full potential all-electron density functional calculations. Chlorine adsorption at the fcc hollow sites is slightly preferred over that at the hcp hollow. The adsorption geometry is in excellent agreement with electron diffraction and ion scattering data. Adsorption energies and surface diffusion barriers are close to those deduced from experiment.

Accepted by Chem. Phys. Lett.

**An *ab initio* Study of α -Al₂O₃(0001):
The Effects of Exchange and Correlation Functionals**

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¹CLRC, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, United Kingdom

²Imperial College of Science and Technology, Prince Consort Road, London

The surface structure of the α -Al₂O₃ (0001) surface has been the subject of a number of investigations which have yielded results which are both qualitatively and quantitatively different. We have re-examined this surface using a variety of calculational schemes implemented within the same computer code; CRYSTAL98. This has enabled us to vary the treatment of exchange and correlation used within the calculation in a systematic manner. Within this approach we have successfully reproduced all previous theoretical predictions of the surface structure of this system. We have also been able to explain the observed variation in the results by highlighting the effects that the choice of exchange and correlation functional has on the ionicity of the surface ions. Despite being able to reproduce and explain all previous theoretical studies, we find that the theoretical results are still at variance with the experimental results, particularly with respect to the contraction of the first to second interlayer distance. Possible reasons for this discrepancy are addressed.

Submitted to Phys. Rev. B

8 Surface Science Related Jobs

Post Doctoral Research Associate in Surface Chemistry and Catalysis

A postdoctoral position is available in the Department of Chemistry at the University of Cambridge.

This position, funded by the European Commission, is available to work under the supervision of Dr. Richard Lambert on fundamentals of heterogeneous catalysis. Experience in the fields of (i) catalyst characterisation and testing or (ii) single crystal UHV techniques is essential.

The position is available from January 1999 for two years and appointment will be on the University's standard scale in the range £ 16,286 to £ 24,479, according to age and experience. Applications including a CV and the names and addresses of two referees should be sent to R. M. Lambert, Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW, UK.

For further information and enquiries contact Dr Richard Lambert via Email: rml1@cam.ac.uk

The University is committed to equality of opportunity. Smoking is not permitted in the Department of Chemistry.

Post-Doctoral Position in Surface Science

A postdoctoral position funded by an EPSRC ROPA award the field of Surface Science is available within the Solid State Chemistry Group at the University of Salford, under the supervision of Professor Martyn E Pemble. The project, which is of one-year duration in the first instance, concerns the use of novel photon-based methods for the study of the formation of ordered films on metal and semiconductor surfaces. Interested persons should contact Prof M E Pemble on +44 (0) 161 295 5296, fax +44 (0)161 295 5272, or by e-mail (m.e.pemble@salford.ac.uk) for further particulars. Further particulars are available online: <http://www.salford.ac.uk/chemist/mepres.html>

Ph.D. Studentship in Surface Science

A studentship is available immediately to support a three-year programme of work leading to a Ph.D. in the Condensed Matter and Materials Physics area (CMMP) in the Physics and Astronomy Department at University College London.

Established in 1994, CMMP has expanded rapidly, and now has roughly 50 members, including about 20 Ph.D. students. The CMMP area consists of both experimentalists and theorists, who have very wide-ranging interests, going all the way from the physics of high-pressure ice to the properties of novel magnetic materials, and from the temperature in the Earth's core to atomic-scale microscopy. This all makes CMMP one of the most exciting and stimulating places in the UK for doing a Ph.D. in condensed-matter physics.

Physics and Astronomy at UCL is one of the leading departments in the UK, with a strong commitment to excellence in both research and teaching. In the 1996 national Research Assessment Exercise, the Department was awarded a grade 5A, a result bettered only by two other departments in the UK.

The Ph.D. studentship available now is not tied to any particular research project, and could be used to support work in any of the many experimental and theoretical projects being done in CMMP. If you are interested and would like to know more, please send an e-mail to Professor Mike Gillan (m.gillan@ucl.ac.uk), who will be delighted to send you further information.

To find out more about the work of CMMP, the Physics and Astronomy Department, and UCL in general, please take a look at the following web pages:

CMMP <http://www.cmp.ucl.ac.uk/>

Physics and Astronomy Department <http://www.phys.ucl.ac.uk/>

UCL <http://www.ucl.ac.uk/>

Postdoctoral Position in Experimental Surface Science at Lund University, Sweden

Applications are invited for a postdoctoral position in surface science in the chemical physics group at the department of chemistry, Lund University, Sweden. The group uses a variety of surface sensitive experimental probes; surface infrared spectroscopy, molecular beam scattering, X-ray photoelectron spectroscopy. The experiments are supported by QM calculations. Work is also performed at the synchrotron at MAX-lab. in Lund. The applicant is expected to work in different projects in collaboration with graduate students and scientists. The projects can be modified and designed according to the applicant's specific scientific interest and experience. Strong background in experimental surface science and ultra high vacuum technique is required. Applicants should submit a CV, a brief description of current research interests and should arrange for three supporting letters. The position is for one year, renewable for a second year and will start in spring 2000.

For further information please contact Dr Per Uvdal, by e-mail (per.uvdal@chemphys.lu.se). Applications should be sent to: Dr. Per Uvdal, Chemical Physics, Department of Chemistry, Lund University, P.O. Box 124, S-221 00 Lund, Sweden.

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