Science outcomes from the use of Grid tools in the eMinerals project

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Abstract

We present a summary of the science outcomes achieved by the eMinerals project so far. The use of Grid computing has allowed us to make progress in a variety of environmentally relevant and computationally demanding problems in mineral physics.

1. Introduction

The purpose of the eMinerals project, one of the NERC eScience testbed projects, is to simulate environmental processes at the molecular level. The eMinerals collaboration includes workers from many different institutions around the UK; we are seeking to pool our expertise and computational resources so as to obtain the maximum benefit from the collaboration. Other papers from the eMinerals consortium describe the management of the project as a "Virtual Organisation" (Dove *et al.*, 2004), and discuss in detail the various tools in hardware, software and middleware that are in use. The purpose of this paper is to summarise the science that has been carried out so far and to show how the work has been enabled by the use of Grid technologies.

The environmentally relevant processes which our simulations address include the weathering and precipitation of minerals, for example sulphides in the problem of acid mine drainage; the absorption of pollutants onto the surfaces of soil particles; and radiation damage processes in minerals used for nuclear waste encapsulation. We also address larger-scale problems in planetary science, such as the composition of the Earth's interior and the crust of Mars, by considering the magnetic properties and pressure-induced phase transitions of iron-containing minerals.

Our simulation techniques include both semi-empirical, classical (potential-based) atomistic modelling and quantum simulations (DFT, Hartree-Fock, hybrid functionals and Quantum Monte Carlo). Classical simulations have smaller computational requirements and are therefore more suitable for investigating large systems (hundreds or thousands of atoms); they also lend themselves to approaches in which many independent simulations are run in parallel. Ab-initio quantum approaches, meanwhile, are capable of handling changes in chemical bonding and oxidation state, and are useful in handling the dissociation of molecules at surfaces, and magnetically ordered systems. When mineral structures are complex or not well known, ab-initio methods may be vital in determining the equilibrium structure of a material, especially as accurate potentials may not be available for the system. It can be particularly fruitful to approach different aspects of a problem with both classical and ab-initio techniques.

Realistic simulations require a very high level of accuracy. Environmentally important processes of adsorption, dissolution and precipitation occur at mineral surfaces, which are often not well characterised. It is therefore necessary to begin by simulating the surface, which often displays relaxations and reconstructions relative to the bulk structure. Water is ubiquitous in environmental processes, and the simulation of hydrous surfaces is orders of magnitude more demanding than simulations *in vacuo*. However, since we find that the hydration of surfaces can dramatically alter their properties, for example altering the relative stability of different surfaces, it is clear that the inclusion of water in our surface calculations is vital if our results are to be environmentally relevant.

Dynamic processes such as radiation-damage effects may require extremely large simulation cells, which in turn requires the use of hardware and software optimised to handle very large systems by parallel processing and efficient scaling.

For all of these reasons, simulations of environmental processes tend to make great demands on our computational resources, both in processing power and in data storage. A principal objective in the development of Grid computing is to make such resources available to users, regardless of their geographical location or institutional affiliation. While this goal is some way from being achieved, we have made progress in the use of Grid tools on the "eMinerals minigrid".

2. Grid tools

We will list briefly the set of tools used so far by the science team. Although many of the technologies are still in development, we are already seeing valuable science outcomes from the use of Grid tools.

2.1 Condor

Condor is a technology that makes otherwise unused compute cycles on desktop PCs available for productive use. It is in use at Cambridge, Bath and UCL. The commonest model so far is the inclusion of large numbers of Windows PCs as compute nodes in a pool with a Linux master node handling job submissions; this is the pattern of the UCL Condor pool, the UK's largest, with over nine hundred PCs. Other Condor pools include heterogeneous architectures and operating systems. The pools make a great deal of processing power available at no additional hardware cost. An issue is that jobs may fail quite frequently due to a node being power-cycled; it is therefore often necessary to perform duplicate runs.

At an early stage it was found that 'porting' scientific codes to the Condor pool depends very much on the programs themselves, especially on the way the executables and input are handled. The surface code METADISE was adapted almost instantly; in contrast, it proved impossible to use Gaussian98 (localised orbitals quantum chemistry), as its Windows versions requires many executables, which Condor does not seem to treat very well. The classical molecular dynamics code DL_POLY was easy to adapt, as was the Plane Wave DFT code ABINIT. Other codes, most importantly the PW-DFT VASP, have proved impossible to compile under Windows.

The setup and management of our Condor resources is described in detail in Wilson (2004), Calleja *et al.* (2004a), and Emmerich *et al.* (2004).

2.2 SRB

The Storage Resource Broker (*SRB*) (Blanshard *et al.* 2004) makes networked storage devices accessible in a seamless fashion; many geographically separate storage devices can be accessed via a single login, and all of the files held on these devices appear as part of a single file system. Various interfaces to the SRB are available, for example the "Scommands" command-line interface for UNIX systems and the inQ graphical file explorer for Windows, which makes navigation of SRB files very intuitive.

The SRB has proved to be a useful aid to productivity, as many of our demanding simulations produce very large quantities of data which must be stored, must remain easily accessible for analysis and for continuation jobs, and which may need to be transferred between several different computing platforms as part of our workflow.

2.3 PIG

The Personal Interface to the Access Grid (*PIG*) system of desktop videoconferencing is in use to improve communication between the members of the project, as discussed in Dove *et al* (2004). The writing of this and other papers has been facilitated by this capacity for both pre-arranged and ad-hoc videoconferencing between members of the project.

2.4 Minigrid

A set of three computing clusters known as the *Lakes* have been constructed at Cambridge, UCL and Bath specifically for eMinerals use. The three clusters are identical, for portability of executables, and provide both processing power and SRB storage space. They are a suitable environment for applications such as VASP which are not suitable for use on Condor resources.

The Lake clusters, the Condor pools and the SRB storage together form the infrastructure of the "eMinerals minigrid" (Calleja et al. 2004b); a pool of diverse computational resources available to certificated members of the consortium. We also make use of general resources such as the HPCx and CSAR supercomputing facilities.

2.5 XML/CML

The use of XML/CML to mark up data sets and represent structures is being championed in the project as a way of standardising data representation and making it easier to transfer information from one program to another (Murray-Rust *et al.* 2004, Wakeline *et al.* 2004).

3. Science results

We here provide an account of the areas in which the use of Grid tools is leading to novel scientific results.

3.1 Goethite: Surface Defects

Goethite is a very common iron oxide mineral and a major component of soil. We use a surface extension of the Mott-Littleton methodology (as implemented in the CHAOS module of METADISE) to study the segregation of various iso-valent cations to the (00.1) and (01.2) surfaces of Goethite (α-Fe_2O_3). A limitation of the CHAOS approach is that it converges slowly with respect to the size of region 1 (which contains the relaxed ions). The use of Condor resources to run many defect calculations in parallel enables us to observe this convergence and extrapolate to determine the system size required for a converged calculation, as illustrated in figure1.
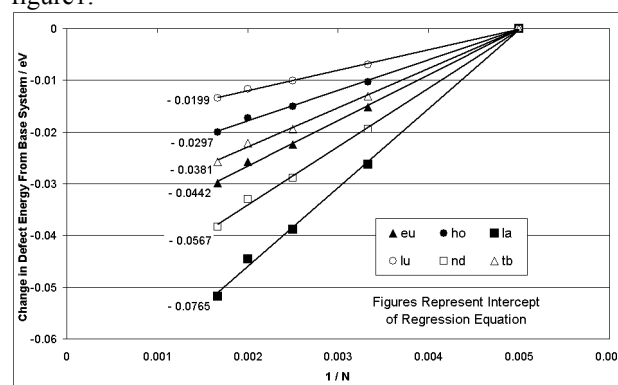

Figure 1: convergence of defect energy with system size for cations on the surfaces of geothite.

The final results (not shown) suggest that size of the impurities has a considerable effect on the magnitude of the segregation energy.

3.2 Calculation of Transmission Coefficients

The water exchange rate in the first hydration shell of cations is of great importance to improve our understanding of the dynamics of hydration. It can be calculated by analysis of the trajectories generated by molecular dynamics simulation (MD), if the water

exchange rate is much faster than the length of the simulation, or otherwise using transition state theory.

In transition state theory, the exchange rate constant is $k=\kappa k^{TST}$ where k^{TST} is the transition state rate constant. The transition state rate constant requires the calculation of the free energy profile of a water molecule leaving the first hydration shell. This is obtained by calculating the ion-water potential of mean force but is beyond the scope of this paper. The transmission coefficient κ is determined from the plateau value of the normalized reactive flux[l].

To compute the transmission coefficient, we first generated a set of starting configurations by running a series of MD simulations using the DL_POLY code, where the separation of the cation to a selected water molecule is constrained to be the transition state distance. We recorded a configuration every 3 ps after a short equilibration period, to obtain 1000 configurations. Then, each configuration was run both backward and forward in time for a short period of time, i.e. 1.4 ps, on the UCL Condor pool. The use of the pool allowed many parallel MD simulations to be performed simultaneously, and since each simulation was independent, failed runs could simply be restarted.

Ion	Direct (s-1)	Calc (s-1)	Exp (s-1)[2,3]
Ca	2.56e10	2.62e10	>1e10
Mg		3.51e5	5.3e5

Table 1. Comparison of water exchange rates in calcium and magnesium hydration shell, as calculated from transition state theory, with direct simulation and experimental data.

3.3 Platinum Sulfide: Lattice Dynamics

Lattice Dynamics (LD) is a computational technique which is used to access the vibrational modes of a system, and from which thermodynamical information can be gathered, via the harmonic approximation (or one of its more refined derivative, like the quasi-hamonic approximation). A well documented requirement for good quality LD is to be able to accurately sample the vibrational Brillouin Zone of a system. Linear Response, as implemented in the code ABINIT, allows the computation of the dynamical matrix at any k-point, at an equivalent cost for each point (a few times more than a simple static point calculation). Increasing the accuracy is then just a matter of increasing the number of calculations. Furthermore, the quality of each calculation is particularly high, as based on Density Functional Theory and taking into account quantum electronic effects.

The Condor architecture is well adapted to this kind of high throughput computing, with no interaction between the many parallel calculations.

Platinum sulphide (PtS) is a little-studied mineral of interest to the mining industry. In Figure 2, we show the dispersion curves of what was thought to be the primitive cell. In fact, a soft mode appears at [.5,.5,0], indicating an instability.

Figure 3 shows the 'doubled' cell, which is stable. The former soft mode is now a low frequency mode corresponding to the low barrier rotation of the Pt atoms around the axis given by the central S atoms. This is thought to be responsible for the peculiar elastic properties of the material, currently under investigation.
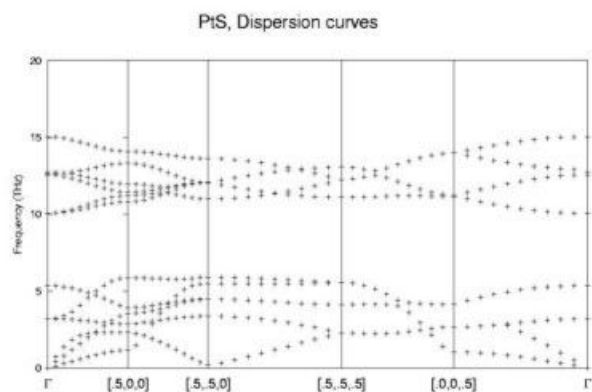

Figure 2: dispersion curves for PtS conventional cell. Note the soft mode at [.5,.5.0].
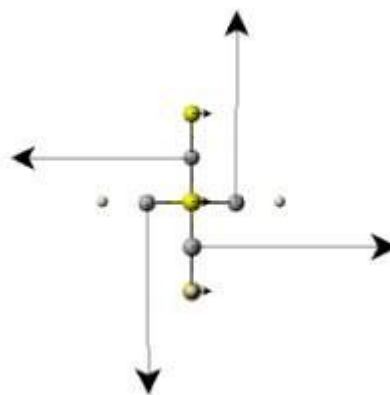

Figure 3: new, stable cell of PtS, showing the eigenvector of the previously unstable mode.

3.4 Diffusion Coefficients in Nanotubes

Nanotubes are fascinating materials, and preliminary studies show that the diffusion coefficients of molecules in them are order of magnitude higher then in zeolites of equivalent size. The potential for nano-chemical-engineeering are important.

Due to the essentially one-dimensional symmetry of the material, the number of molecules in a typical simulation box (periodically repeated) is small. While it is usual in the field of molecular modelling to use as small a system as possible, the diffusion coefficient converges quite poorly with the size of the system. There are two ways of obtaining reliable diffusion coefficients: increasing the system size and thus the resource requirements, or increasing the number of systems. This second options is advantageous as the computational cost increases linearly with the number of calculations and very modest resources can cope with the smaller system. An added bonus is that the statistical error on the result is readily available.

A set of one thousand similar systems was generated, and the corresponding trajectories were generated on the UCL Condor pool using DL_POLY. The statistical analysis was also carried out using Condor facilities.

To illustrate the method, we present the statistical distribution of coefficients for Ar atoms diffusing in a 19:0 carbon nanotube at a pressure of .5 kB in Figure 4.
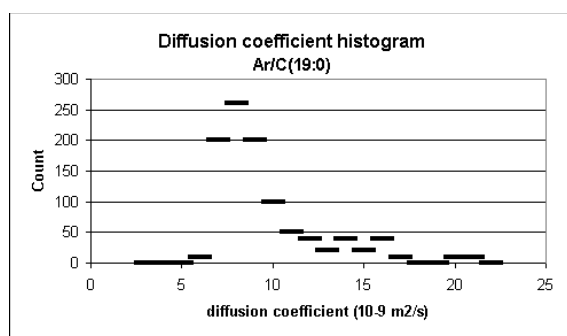
Figure 4: distribution of diffusion coefficients for Ar in a carbon nanotube.

Diffusion coefficient of other particles, under various conditions of temperature and pression are being investigated.

3.5 Calcite

Calcite, $CaCO_3$, is the primary constituent of minerals such as chalk, limestone and marble. Under ambient conditions, it has a crystal structure that consists of alternate layers of calcium cations and carbonate molecular ions, as shown in Figure 5.
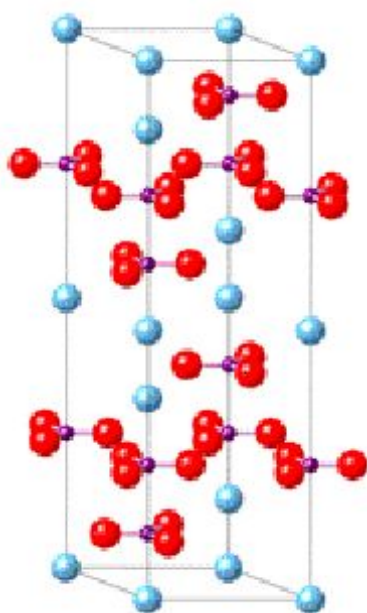

Figure 5: structure of calcite.

Diffraction measurements suggest that on heating the carbonate groups begin to rotate. The same experiments suggest that there is a change of phase at 1260 K to a structure in which the orientations of the carbonate molecular ions are disordered with respect to each other. Studying calcite at high temperature is experimentally difficult as the carbonate ions dissociate. Although this process can be inhibited by application of pressure, it has not been possible to heat samples into the high-temperature disordered phase. Computer simulation is therefore the only approach that can give information about the behaviour in the high-temperature phase.

We have performed molecular dynamics simulations of calcite to investigate the phase transition, using the DL_POLY code, carrying out a series of simulations for many temperatures over a range of pressures. Each single calculation took of order 12–24 hours running time. By using both the UCL Condor pool and eMinerals minigrid resources, we were able to generate the several hundred data points shown in figure 6, compared to 10-20 points for a typical computational study. This allows us to observe small effects such as the inflexion in the volume at the phase transition, which in this simulation occurs at 1780 K, as shown by the disappearance of the (113) peak intensity.

The observation of a large thermal expansion at higher temperatures is a new result, and is contrary to previous expectations. We now interpret this as arising from out-of-plane rotations of the carbonate molecular ions.
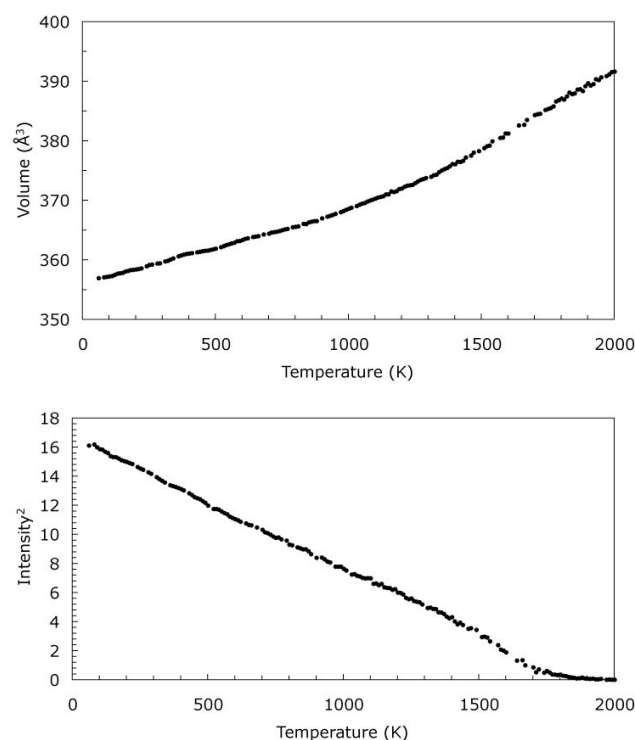

Figure 6: Simulation data showing phase transition in calcite.Above, cell volume, below, (113) peak intensity[2].

3.6 Radiation damage

Materials used for the immobilisation of radioactive waste will inevitably suffer damage from decay events, with most of the damage resulting from the recoil of uranium atoms during alpha-decay events. Key questions in the selection of waste form materials are the resistance of the material to amorphisation by this damage, and the effect of damage on the rate at which radioactive nucleides diffuse out of the waste form into the environment.

By using the DL_POLY molecular dynamics code with simulation boxes containing several hundred thousands of atoms, we can observe the effects of a decay event.

Figure 7a shows the aftermath of a decay event in zircon; a low-density depleted region is surrounded by an amorphous cloud consisting mostly of polymerised silica, the whole cloud containing about 5000 atoms. Two adjacent decay events (figure 7b) can result in the overlap of depleted regions. This allows for the interpretation of experimental data on diffusion and volume swelling in damaged zircons on the basis of two percolation thresholds, the first at an amorphous fraction of 0.3 corresponding the percolation of amorphous regions and

the second at a fraction of 0.7 corresponding to the percolation of depleted regions; each threshold is marked by an increase in diffusion.[4]
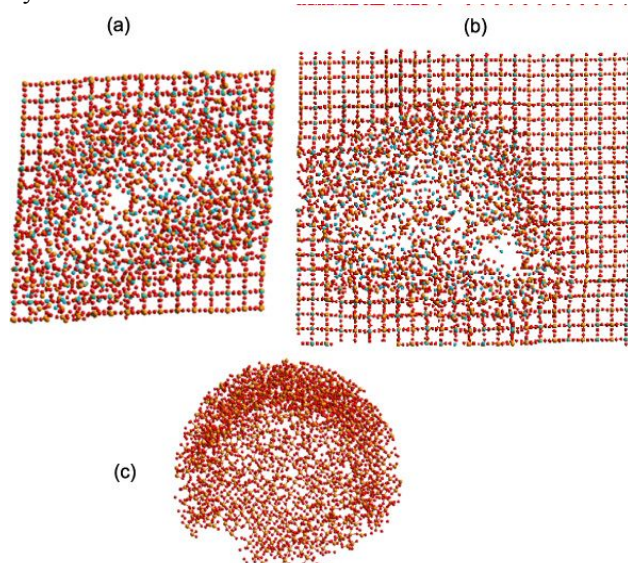

Figure 7: DL_POLY simulations of alpha-decay damage in zircon.

Figure 7c, showing the polymerised Si-O phase in the amorphous region, sheds light on the vexed question of the resistance of materials to amorphisation by radiation damage; it appears that materials capable of forming strong covalent (short-range) bonds are readily amorphised, while those in which longer-range (ionic) forces are dominant are resistant to radiation damage as they do not form amorphous covalent networks. This is illustrated by the pyrochlore system $Gd_2(Zr_xTi_{2-x})O_7$, in which the resistance to amorphisation correlates directly with the proportion of the highly ionic Zr-O phase[5].

3.7 Clays

Research is under way using the SIESTA ab-initio code to study the interaction of organic pollutant molecules such as DDT, dioxins and biphenyls with soil minerals. Preliminary calculations on the adsorption of tetrachlorodibenzo-p-dioxin on the dry surface of pyrophyllite have been carried out using Condor resources at Cambridge and UCL.

The combinatorial problem posed by the large number of candidate organic molecules and clay minerals is discussed as a workflow issue in Wakeline *et al.* (2004). Since this is another system where the environmentally relevant interactions will occur in the presence of water, figure 9 illustrates the simulation of hydrous clay surfaces using SIESTA.
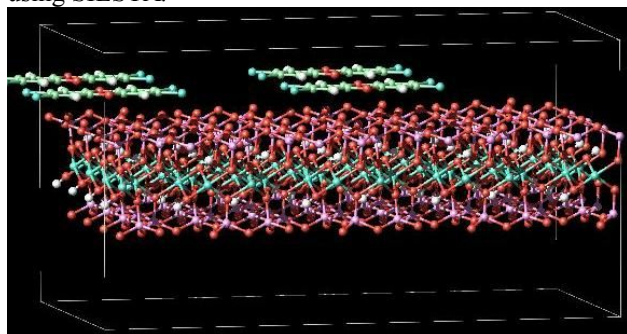

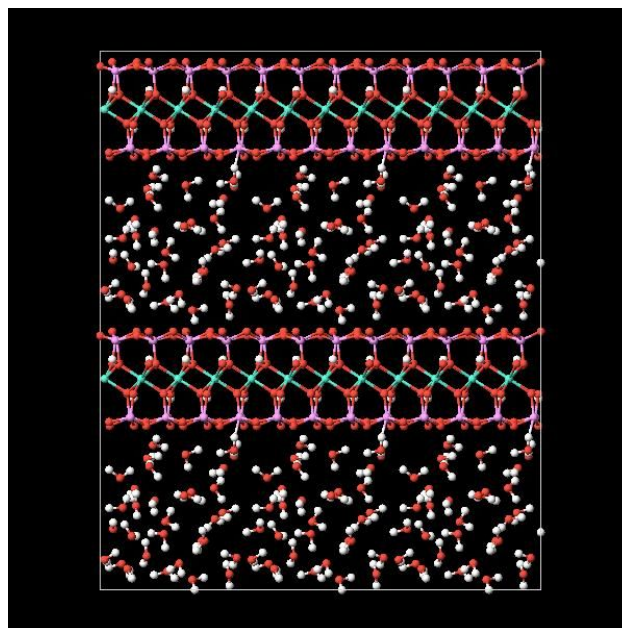*Figure 8: a dioxin on the surface of pyrophyllite clay.*

Figure 9: SIESTA simulation of hydrous clay surfaces

3.8 Hydrous Silicate Surfaces

We have employed a range of complementary computer modelling techniques to study silicate/water interfaces. *Ab initio* calculations based on density functional theory using the VASP plane-wave code were used to investigate chemical bonding and the electronic structure of hydrated quartz surfaces, while information on lowest energy structures, water adsorption and dissolution energies of silica nano-tubes were obtained by classical static lattice methods (METADISE). Finally, multi-layer adsorption of water at quartz surfaces and the effect of temperature were investigated using classical molecular dynamics simulations (DL_POLY). The DFT calculations of the structures and stabilities of two (0001) a-quartz surfaces and their affinity for water have shown that, in vacuo, the fully coordinated surface containing surface O-Si-O bridges and planar six-rings is more stable than the under-coordinated surface, where the surface silicon and oxygen atoms are terminated by dangling bonds. Upon hydration, these stabilities are reversed with the formerly under-coordinated surface, where the dangling bonds are now terminated by OH groups, by far the more stable of the two. These results suggest that in the presence of water the hydroxylated surface would be dominant.

Associative physisorption of water occurs on the fully coordinated surface with a decrease in stability of the surface, whereas dissociation of water leading to a fully hydroxylated surface (figure 10) is the preferred mode of adsorption at the dangling bonds of the under-coordinated surface, increasing the coordination and local geometry of the surface species to resemble the bulk environment.

A similar trend is shown in the classical simulations of a silica nano-tube, where the tube walls containing fully coordinated species linked by O-Si-O bridges are fairly resistant towards attack by water, as the non-destructive associative physisorption of water is unlikely to be followed by dissociative adsorption with consequent breaking of Si-O bonds, which is energetically not much more favourable. However, at the ends of the tube, not only is the initially strained environment of the end-ring in the anhydrous tube highly reactive towards water, but also

the structure is easily attacked even further by dissociative chemisorption of water and possibly replacement of silicons by protons (figure 11). From our calculations it is clear that long nano-tubes or closed structures will be significantly more resistant against dissolution than short open-ended structures.
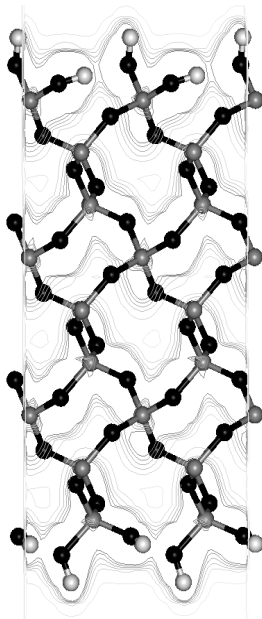

Figure 10: dissociative adsorption of water on an under-coordinated surface, leafing to hydroxylation.
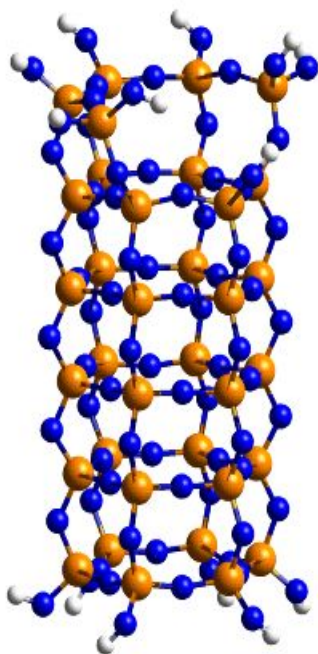

Figure 11: Geometry optimized structure of the hydrogen-capped nano-tube with one Si dissolved from the structure (Si = yellow, O = blue, H = white).

Initial results from classical Molecular Dynamics simulations of the same quartz surfaces with multi-layers of liquid water suggests that the fully-coordinated surface allows penetration of water molecules into the channels of the bulk crystal structure, which occurs more rarely when the surface is terminated with hydroxy groups. In addition, we observe a clear low-density region between the dissociatively adsorbed water layer at the surface and the molecular water further away from the surface, which has the structure of bulk liquid water.

This work, showing the interplay between electronic structure calculations and potential-based techniques, is a clear example of the benefits derived in employing complementary methods to identify and investigate important surface features and reactivities.

3.9 FeO

We are studying the phase transitions as a function of pressure in Fe-bearing minerals, using high-level first principles calculations. It is found that traditional density functional theory (DFT) calculations fail to reproduce systems containing highly localised d- and f-electrons, including iron oxide minerals. This failure of DFT is related to the insufficient cancellation of the electron self-interaction in the local exchange functional. We attempt to remove the improper self-interaction correction by making use of the exact cancellation between the Coulomb and exchange terms in Hartree-Fock theory, *i.e.* to use hybrid DFT exchange functionals[6].

We have now extended this study to model the structural and magnetic phase transitions in FeO for a number of different hybrid Hamiltonians. We have undertaken a systematic study, mixing the exchange functionals of Becke and Hartree-Fock (Fock-exchange) to understand how the amount of Fock-exchange changes the phase diagram of wüstite.

To scan the phase diagram of one compound is often computationally expensive, as it involves performing calculations at a range of pressures for all the possible magnetic and geometric polymorphs. For some compounds we are required to perform between 50-100 calculations to determine the phase diagram solely as a function of pressure. If we also want to take into account the effect of the Fock-exchange, the number of calculations can easily increase to thousands. Prior to the availability of the computers in the E-minerals mini-grid it could take several years to do a detailed determination of the phase diagram for one mineral.

This is an excellent application for Condor resources, as it involves many independent runs which can all be submitted simultaneously, and we have therefore taken advantage of the UCL Condor pool. The data produced is stored in the SRB for ease of access.

At ambient temperature and pressure wüstite (FeO) crystallises in an anti-ferromagnetic (AFM) B1 structure, but as the temperature is decreased it undergoes a structural phase transition to a rhombohedrally distorted B1 structure (r-B1). However, the effect of pressure is less well understood. It has been suggested that the B1 polymorph transforms into a B8 polymorph, but it has been difficult to determine, whether the high-pressure polymorph is a normal B8 or an inverse B8 (i-B8) structure; it has also been suggested[7] that the B8 and the i-B8 structures might co-exist. However, from computational studies the i-B8 structure is found to be slightly more energetically stable than the B8 structure. All calculations predict the high-pressure structure to be anti-ferromagnetic. There have been experimental predictions that there is a magnetic transition at pressures of ca. 120 GPa, *i.e.* suggesting that the anti-ferromagnetic structure becomes non-magnetic. By performing calculations with the CRYSTAL03 code we have been

able to predict the phase diagram of wüstite as a function of pressure. Our calculations propose that at T=0 K we observe two phase transitions, as shown in Figure 12: at around 80 GPa the r-B1(AFM) structure transforms to the i-B8(AFM) structure, which at pressures higher than 145 GPa undergoes a second phase transition to the B8(NM) structure. Hence, the latter phase transition is also associated with a magnetic spin collapse.
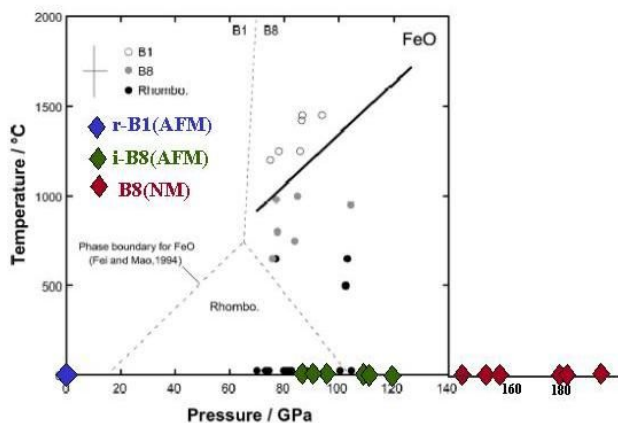

Figure 12: phase diagram of FeO.

3.10 IRON SULPHIDE

We have been examining magnetostructural effects in FeS troilite and pyrrhotite using the VASP plane-wave code. Troilite has an unusual structure, crystallising in the space group (P -6 2 c) – apparently the only mineral to do so. It is a derivative of the NiAs structure, with a large (24 atom) unit cell. Previous simulations using DFT have not obtained values of the c/a ratio consistent with experiment. Magnetostructural effects due to the antiferromagnetic ordering of iron moments along the c axis appear to be important in determining the structure and properties of troilite.

By running our simulations at very high accuracy (500 eV plane-wave cut-off, k-point grid 6*6*4, using GGA with the PW91 functional and the spin interpolation of Vosko, Wilkes and Nussair) we have been able to obtain an accurate simulation of the structure and properties of troilite. Comparison with a nonmagnetic simulation reveals the importance of the magnetostructural effects.
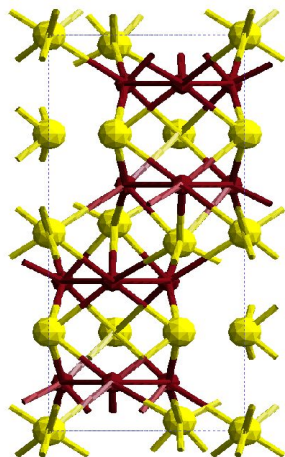

Figure 13: troilite structure viewed down [010], showing Fe in red and S in yellow.

Parameter:	Experiment (8)	Prior sim. (9)	Our sim (AFM)	Our sim (Non-magnetic)
a (Å)	5.96	5.98	5.95	5.86
c (Å)	11.75	11.23	11.65	10.47
c/a	1.97	1.88	1.96	1.79
K (GPa)	73-82	75-80	75	-

Table 2: structural properties of troilite, showing the importance of magnetic interactions.

This executable is not available on the Condor resources and is best used on a parallel cluster; most of our calculations use 16 processors in parallel. Our initial simulations were carried out on HPCx. We are now investigating the pressure phase diagram of troilite using CSAR resources, while on the eMinerals Lake resources we are simulating 4C-pyrrhotite (Fe_7S_8), which is obtained from a supercell of the troilite structure by ordering of Fe defects; this ordering makes the material ferrimagnetic.

The SRB has proved invaluable due to the need, not only to store large charge and wavefunction files for later analysis, but also to transfer the work from one platform to another. The transfer of pyrrhotite calculations from HPCx to Lake resources involved moving restart files of up to 4Gb in size. Using the SRB this could be accomplished seamlessly.

Conclusions

We have presented results from a wide variety of environmentally relevant simulation problems, demonstrating that the use of Grid resources is now allowing us to obtain useful results faster and more accurately than was previously possible. The pooling of resources using Condor has led to a tremendous increase in productivity for situations requiring large numbers of relatively small jobs to be run independently. The Lake clusters provide an environment for large jobs requiring parallel processing. Data storage and transfer using the SRB has simplified data handling and workflow, helping us to cope with the large volumes of data resulting from our newly increased productivity. As we continue to move towards full Grid computing we look forward to an ever-accelerating pace of discovery.

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