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3 Computational Modelling of Inorganic Solids

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5 This report covers papers published in 2010 dealing with the application of computational techniques to inorganic solids. It deals mainly with continuous solids that are ionic in nature; work on metals, MOFs and surfaces is excluded. Special attention is given to solids used in solid oxide fuel cells, multiferroics, iron-based superconductors, nanostructures and
 10 systems relevant to biominerals and earth science.

Highlight

One paper stands out because it is concerned with traditional inorganic chemistry¹. The authors were interested in extending the chemistry of Ag(II) motivated by the previously noted possibility that argentofluorates could be superconducting. As AgF₂
 15 is very difficult to make under high pressure and AgO disproportionates to give Ag(I) and Ag(III), the authors turned to the sulfate. They studied 20 polymorphs of AgSO₄ including those with Ag(I)/Ag(III) and those containing S₂O₈²⁻. They concluded that AgSO₄ should be a true paramagnetic salt of Ag(II), but that the potential for the appearance of high T_c superconductivity is low.

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1. Introduction

Several journals have produced themed issues in this area during 2010. Physical Chemistry Chemical Physics volume 12 issue 30 was on ‘Solid State Structure
 25 Prediction’ and Journal of Materials Chemistry volume 20 issue 46 on ‘Modelling of Materials’. Volume 22 Issue 38 of Journal of Physics – Condensed Matter had a section on ‘Theory meets Industry’. A special Issue of Molecular Physics on ‘Electrons, Molecules, Solids and Biosystems:Fifty years of the Quantum Theory Project’ included an overview of the evolution of the WIEN2k code². A useful
 30 article in Angewandte Chemie³ outlined the use of quantum chemistry in calculating the thermochemistry of solids illustrated by a number of well-chosen examples. Volume 71 of Reviews in Mineralogy and Geochemistry consists of a series of articles based on a course on Theoretical and Computational Methods in Mineral Physics held in December 2009 prior to the meeting of the American Geophysical
 35 Union.

The trend towards the increasing use of ab initio techniques continues. The use of the addition of a Coulomb term to take account of electron repulsion on the metal ion (+ U method) is now in widespread use for strongly correlated systems such as transition metal oxides. Hybrid functionals are also used for this purpose. Imada and
 40 Miyake⁴ discussed progress in methodologies for strongly correlated systems. I foresee an increase in the inclusion of spin-orbit coupling in calculations. Systems

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with canted spins, for example many iron-containing oxides, require spin-orbit coupling to correctly describe the spin arrangement. As spin canting plays a role in type II multiferroics (see section 2.3), these materials will need spin-orbit coupling for their proper description. There may be other advantages in including this coupling as illustrated by a recent study of FeCO_3 ⁵ in which it was found necessary to obtain agreement with the observed magnetic properties. For layered structures, the addition of van der Waals interactions can stabilise the structure as shown by Londero and Schroder⁶ for V_2O_5 . Schemes to calculate excitations in materials are being developed^{7, 8}. The latter paper used a Wannier function approach. Maximally localised Wannier functions are also used in EPW⁹, a program to calculate electron-phonon coupling.

Nonetheless, there are still meaningful results to be obtained from interatomic potential calculations. The presence of isolated charged defects is something that can easily be explored using such methods but difficult for ab initio periodic methods. In addition avoidance of prohibitive computer resource use can still make this the preferred method for molecular dynamics and genetic algorithm calculations. Increased use of these last two types of calculation continues^{e.g. 10,11,12} as they can give information on Gibbs energies, ΔG , rather than simply energies at 0K. Despite the large amount of resource acquired, even in this area quantum methods are now being used, for example a quantum Monte Carlo study of silica¹³.

At the time of the last report, solids exhibiting colossal magnetoresistance (CMR) were a focus of much research. However lack of applications for such materials has led to a slowing down of interest. Currently, hot topics are multiferroics (materials possessing two or more cooperative properties) and iron-based high T_c superconductors.

An area attracting a lot of interest is solids used, or of potential use, in fuel cells. This is an area where theory can play a major role in elucidating diffusion paths and mechanisms.

Properties and structures of zeolites were an early example of the power of interatomic potential methods. There is still a steady stream of papers on this topic and in particular on the interaction of molecules with zeolites, but many nowadays use ab initio methods.

Computation is increasingly used in mineralogy and biomineralisation and, in this Report, I include examples from these fields, including a paper¹⁴ addressing the important question of the origin of the water on Earth. Finally I consider calculations on nano structures. I am not including surface calculations, although the modelling of molecules on surfaces and nanoparticles is a lively area of research and of importance to understanding heterogeneous catalysis. Neither shall I cover calculations on metals, alloys or amorphous materials.

2 Oxides

2.1 Perovskites

The versatile perovskites continue to attract much interest. In this section, I consider studies of perovskites and post-perovskite structures other than those that are dealt with as examples of solids having properties of high current interest such as multiferroics.

Since electronic and magnetic properties are often of interest for this class of

compounds, there have been many studies using DFT methods. Hamdad and Bouhafs¹⁵ employed both LDA (LDSA) and GGA methods with and without the addition of a +U term to study the electronic and magnetic properties of CaMnO₃.
95 Unsurprisingly they found that GGA + U gave more accurate results than the other methods. Goncalves et al¹⁶ calculated the electric field gradient in CaMnO₃ and Cd-doped CaMnO₃ at the Ca atom. Iorgulescu et al¹⁷ used DFT calculations to support their experimental work on Ba₈Co₂Mn₆ClO₂₂. Matar et al¹⁸ have studied perovskite and post-perovskite CaRhO₃. Natsui et al¹⁹ have used DFT calculations to conclude
100 that the oxygen defect energy and hence the activation energy for oxide diffusion is smaller for the hexagonal form of BaTiO₃ than for the cubic form. Liu²⁰ et al have studied BaHfO₃ using LDA. Cherrad et al have also used LDA to study SrHfO₃²¹ and CaHfO₃ and CaSnO₃²². Sesion et al²³ studied CdSnO₃ using both LDA and GGA and showed that GGA produced a more accurate optimised geometry. Barboza et al²⁴
105 employed both LDA and GGA to study CdGeO₃. Zhang et al²⁵ report GGA + U calculations on SrKFeWO₆. Bjorheim et al²⁶ have used DFT calculations to obtain hydration enthalpies of zirconates, MZrO₃ where M = Pb, Ca, Sr, Ba.

Interatomic potential methods are useful for perovskites when the interest is in mechanical or thermal rather than electronic or magnetic properties as illustrated by
110 the calculations of Steele et al²⁷ which relate the variation in mechanical and thermal properties in perovskites, ABO₃, to tilting of the BO₆ octahedra. The degree of tilting is linked to the relative sizes of A and B ions.

2.2. Materials for Solid Oxide fuel cells

Modelling studies of both electrode and solid electrolyte materials for fuel cells have
115 been published. DFT calculations are increasingly used in this area but it remains one where interatomic potential calculations still give valuable insights.

An issue of Philosophical Transactions of the Royal Society A on the theme of 'Energy Materials to Combat Climate Change' contains a comprehensive review of the application of computational methods to materials including those for hydrogen
120 production and storage, energy storage and conversion and emission and absorption of light²⁸. A number of applications are described using both ab initio and interatomic potential approaches. In the same issue, Islam²⁹ reviews the role of modelling techniques applied to novel materials for lithium batteries and solid oxide fuel cells. Malavasi et al³⁰ have written a critical review of oxide- and proton-
125 conducting electrolyte materials which includes examples of the application of computational techniques to the conduction mechanism.

Tealdi et al¹⁰ have used interatomic potential calculations and molecular dynamics to study the defects and oxide ion conductivity mechanism in the melilite-type LaSrGa₃O₇. Hooper et al¹¹ used interatomic potentials and the genetic
130 algorithm technique to study ionic conductivity in samarium-doped ceria, a promising electrolyte, containing a high concentration of samarium. This enabled them to put forward an explanation for the high conductivity at low concentrations and the drop-off at concentrations >11%. Yu et al¹² used atomistic simulation and molecular dynamics to explain the observed changes in ionic conductivity of
135 scandium-stabilised zirconia thin films. Ye et al³¹ have studied the diffusion of nickel from the substrate through Gd-doped ceria films. In the themed issue of Journal of Materials Chemistry, 'Proton Transport for Fuel Cells', Islam's group presented atomistic simulations on the proton conductor BaZrO₃ and potential proton conductor BaPrO₃³². This group have also studied defects and protonation in

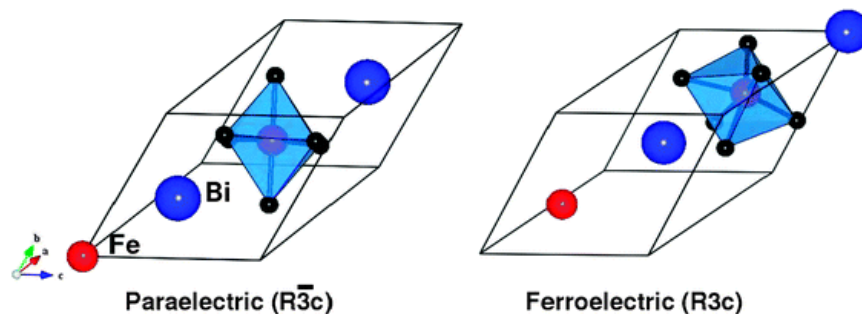
140 LaNbO_4 ³³ and in silicon- and germanium-based apatite ionic conductors³⁴. Kushima and Yildiz³⁵ used DFT to obtain oxygen migration paths and barriers in yttria-stabilised zirconia and then considered the barrier energies as a function of strain. They conclude that inducing optimal strain can lead to high ionic conductivity at reduced temperatures.

145 As well as solid electrolytes, electrode materials have been the subject of calculations. Armstrong et al³⁶ have used DFT calculations to look at lithium coordination sites in the promising anode material Li_xTiO_2 . Gardiner and Islam³⁷ reported on atomistic calculations of defect and transport properties in the possible cathode material $\text{LiFe}_{0.5}\text{Mn}_{0.5}\text{PO}_4$. The lowest energy intrinsic defect was found to
150 be the cation antisite defect with exchange between Li and Fe/Mn. Mastrikov et al³⁸ have used DFT calculations to obtain the electronic structure of- and formation of - oxygen vacancies in $\text{Ba}_{1-x}\text{Sr}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$. Naumovich et al³⁹ have studied oxygen ion transport in $\text{La}_2\text{NiMO}_{4+\delta}$ ($M = \text{Fe}, \text{Co}, \text{Cu}$) and showed that doping with M^{3+} leads to higher a higher concentration of charge carriers but a decrease in anion
155 mobility. Shishkin and Ziegler⁴⁰ have studied H_2 and CH_4 activation on the surface of ceria using a model of an Ni/ CeO_2 anode.

2.3. Multiferroics

The multiferroics that have attracted most interest both experimentally and
160 theoretically are those with cooperative electric and magnetic properties. Such multiferroics can be divided into two classes. In type I, ferroelectricity and ferromagnetism or antiferromagnetism are both present in the solid but arise from different structural features. In general there is little coupling between the two effects. In type II multiferroics, ferroelectricity and ferro- or antiferro-magnetism are
165 closely linked, so that, for example, application of a magnetic field will cause the solid to be ferroelectric.

The most studied example of a type I multiferroic is bismuth ferrite, BiFeO_3 , which is ferroelectric and antiferromagnetic at room temperature.



170 Figure 1 Paraelectric $R\bar{3}c$ and ferroelectric $R3c$ phase of BiFeO_3 in the rhombohedral setting. Black spheres are oxygen atoms. The octahedron centred at one Fe atom is shown. Note the off-centering of the Fe atom and the corresponding octahedra distortion. The origin of the ferroelectric structure has been shifted for clarity (from reference 41)

The most well-known example of a type II multiferroic is terbium manganite.
175 Stroppa and Picozzi⁴¹ have undertaken a detailed study of typical type I and type II multiferroics using hybrid-DFT. They found that the HSE hybrid functional provides a good description of the structural, electronic and magnetic properties of their test

solids, BiFeO₃ and HoMnO₃, but pointed out that the percentage of exact exchange used may need to vary with the material studied. This group have also studied the
180 multiferroic phase of DyFeO₃⁴² and suggest that Fe-Dy coupling is mediated by overlap of Dyd and O2p. The multiferroic properties of BiFeO₃ are enhanced if the material is in the form of a thin film. Wojdel et al⁴³ have reported LDA + U calculations on BiFeO₃ films under strain and conclude that, by inducing structural softness, very large magnetoelectric effects could be obtained. Lee et al⁴⁴ have used
185 DFT calculations to study the effect of La-doping on the properties of BiFeO₃ and Zhang et al⁴⁵ have studied the effect of doping with Sc³⁺, La³⁺ and Y³⁺. Feng⁴⁶ predicts that Bi₂FeNiO₆ will be ferroelectric and ferrimagnetic. Shanavas et al⁴⁷ have investigated MnWO₄, reproducing the correct magnetic ground state and showing that the ferroelectricity is due to spin-orbit coupling. Kumar et al⁴⁸ predicted that
190 Y₂NiMnO₆ will be multiferroic. Fechner et al⁴⁹ present ab initio calculations that lead to the proposal that a composite material consisting of a thin film of magnetic solid such as Fe laid on the surface of a ferroelectric material (ATiO₃ where A = Pb, Ba) would form a robust type II multiferroic.

2.4. Oxides

195 Simple oxides continue to provide new insights. Sokol et al⁵⁰ used DFT calculations on supercells to investigate O atoms as a defect in α -Al₂O₃. They found that upon allowing the structure to relax, the interstitial O atom displaces a neighbouring oxide ion such that the two oxygens are only 1.44 Å apart, a distance characteristic of the peroxide ion, O₂²⁻. The calculations also showed transfer of charge from the oxide
200 ion to the interstitial atom. The occurrence of peroxide defects has formerly been reported for MgO, ZnO(wurtzite) and SnO₂(rutile). It was suggested that this could have implications for interstitial O in other close-packed structures. This is particularly interesting due to the increasing number of papers dealing with neutral defects in crystals. Such defects are more easily handled using periodic calculations
205 than charged defects.

Labidi et al⁵¹ presented calculations on the MgO/SrO system and found deviations from Vegards Law. Dai et al⁵² illustrated the feasibility of using interatomic potential methods to study piezoelectricity in nanoparticles of ZnO and Botello-Mendez et al⁵³ have used DFT calculations to explore the effect of carbon- and sulfur-doping
210 on ZnO nanostructures. Palacios et al⁵⁴ have used DFT + U to study the electronic structure and optical properties of ZnO doped with Co and Cd. Rozale et al⁵⁵ have used the accurate FLAPW DFT with LDSA to study Co-doped ZnO and consider the effect of altering the value of U. Blanca-Romero et al⁵⁶ have studied Eu-doped ZnO, in particular the relaxation of O atoms surrounding Eu. Gorbunova et al⁵⁷ have used
215 DFT to study the effect of Li and Na incorporation in BeO and found that BeO remained non-magnetic after incorporation of Li but there is a magnetic moment on the incorporated Na. Roquefelte et al⁵⁸ have studied the temperature dependence of properties of CuO using hybrid DFT. The effect of temperature was modelled by introducing ferromagnetic domains into the antiferromagnetic structure to mimic the
220 changes in the local symmetry of the spin density. Stausholm-Moller et al⁵⁹ investigated interstitial Ti, O vacancies and H incorporation in TiO₂ using DFT + U. They show that for U = 2.5 eV for Ti, excess electrons are localised at Ti sites and appear as states within the band gap of pure TiO₂ in fair agreement with observation. Shirley et al⁶⁰ used DFT calculations to study properties of Al-doped TiO₂. They
225 found that Al increases the band gap and that at industrially relevant temperatures

migration of Al through the crystal is only possible for the rutile polymorph. Kamisaka et al⁶¹ reported DFT calculations on Nb- and W-doped TiO₂ as anatase. In the case of W doping, they found that the substitution is stabilised by one or two adjacent oxygen vacancies. Shen et al⁶² have studied intrinsic vacancies in cubic
230 ZrO₂ concluding that a Schottky defect is favoured for the bulk and an O atom vacancy at the surface. Borges et al⁶³ have studied the electronic, vibrational and optical properties of SnO₂. Loyala et al⁶⁴ have used interatomic potentials to study the vibrational properties of γ -Al₂O₃. Grau-Crespo et al⁶⁵ have studied the electronic structure of γ -Fe₂O₃ and the ordering of Fe vacancies and concluded that the
235 vacancies should be fully ordered at equilibrium. Zhang et al⁶⁶ have used molecular dynamics to study the dehydration of goethite (α -FeOOH) to hematite (α -Fe₂O₃). Knot'ko et al⁶⁷ used interatomic potential calculations to obtain defect energies and defect mobilities in ZrO₂-based solid solutions, NiO and CdO.

Ylvisacker et al⁶⁸ have examined the orbital ordering and magnetic properties in
240 the peroxide RbO₂. Tapilin et al⁶³ used LSDA DFT calculations to study SrCoO_x with $x = 3, 2.875$ and 2.75 . They found that all three solids have metallic conductivity, but as LDA is known to underestimate band gaps, it could be worth checking whether this remains true for +U or hybrid calculations. Carlier et al⁷⁰ used DFT and DFT + U to investigate the spin density on Li in Li₆CoO₄ in order to throw
245 light on the observed ⁷Li MAS NMR spectrum of this compound which showed two very different chemical shifts for the two distinct Li sites. Dalverny et al⁷¹ showed, using DFT + U calculations, that the peculiar structural behaviour of CoO below the Néel temperature is the result of the interplay between magnetic and orbital ordering.

250 Inerbaev et al⁷² have studied oxygen vacancy formation in nanocrystalline CeO_{2-x}. Chen et al⁷³ have studied Zr-doped ceria and Wang et al⁷⁴ have studied Ni-doped ceria. Xu et al⁷⁵ have assessed interatomic potentials for elastic properties of CeO₂.

Yeon et al⁷⁶ have identified new polar oxides A₃V₅O₁₄ (A= K, Rb, Tl) with a layered structure of corner-sharing VO₄ tetrahedra and VO₅ square pyramids.

255 With increasing computer power, calculations taking account of entropy due to disorder as well as energy are appearing more often. Seko⁷⁷ has reviewed methods using DFT and cluster expansion and illustrated this with a phase diagram for ZnO/MgO, cation disorder in MgAl₂O₄ and SnO_{2-x}. Hooper et al⁷⁸ have used a DFT-based genetic algorithm method to study lanthanide-doped ceria.

260 Studies of incorporation of radionuclides into solids can aid in the choice of a material for storing nuclear waste. Shuller et al⁷⁹ have studied Np in studtite ([UO₂(O₂)(H₂O)₂].2H₂O). Studtite may form from spent fuel rods. Ryzhkov et al⁸⁰ used interatomic potentials to determine the geometry around the defect when Pu³⁺ and Pu⁴⁺ substitute for Zr in zircon. Gryaznov et al⁸¹ have looked at helium
265 incorporation into UO₂, PuO₂ and MOX(solid solution of UO₂ and PuO₂) using DFT + U calculations. They conclude that incorporation of He is exothermic. Chartier et al⁸² have studied the stability of xenon clusters in UO₂ and Govers et al⁸³ have studied the incorporation and migration of Xe atoms in UO₂. Both studies employed interatomic potentials. Bishop et al⁸⁴ reported molecular dynamics calculations on
270 displacement cascades in UO₂. Such cascades arise when the very strong irradiation leads to defect centres due to atom displacement.

Studies of parameters for ab initio and interatomic potential calculations on solids relevant to the nuclear industry have been reported. Liu et al⁸⁵ identified a value of U for DFT + U calculations on δ -Pu and PuO that gives correct structural and

275 electronic properties. Read and Jackson⁸⁶ have derived enhanced potentials for calculations on UO_2 .

Goel et al⁸⁷ have studied the important solid state laser material YAG (yttrium aluminium garnet). They were particularly interested in phonons in this material and the effect of pressure on phonon frequency.

280 3. Oxyanion and non-oxide systems

3.1. Solids containing oxyanions

In this section I cover solids containing discrete oxyanions such as carbonate, oxalate and sulfate but also some solids which could be described as complex oxides but do not fit into any of my other categories.

285 Badaut et al⁸⁸ report a very interesting study of siderite, FeCO_3 . Experimentally, siderite is an antiferromagnetic insulator. However DFT calculations give a very small energy gap between the ferro- and antiferro-magnetic states and give the ferromagnetic state at lower energy. In order to reproduce an antiferromagnetic ground state, the authors find it necessary to include spin-orbit coupling. Matar⁸⁹ has studied uranyl carbonate UO_2CO_3 and find it to be an ionic-like semiconductor. 290 Vinograd et al⁹⁰ used atomistic simulation to calculate the thermodynamics of mixing in the carbonate solid solution $(\text{Ca}_x\text{Mg}_y\text{Mn}_{1-x-y})\text{CO}_3$.

Matar et al⁹¹ investigated the relative stabilities of the β , α and ω phases of MgMoO_4 and NiMoO_4 and concluded that for Mg the order of stability is $\beta > \alpha > \omega$, 295 the reverse is true for Ni. They attribute this to the greater covalent nature of the Ni-O bonding. Xu et al⁹² have used DFT to study defects in LiNbO_3 . Several aspects of phosphates have been studied. Jay et al investigated possible structures for β - $\text{Ca}_3(\text{PO}_4)_2$ in particular the distribution of vacancies on the partially occupied Ca(4) site. Koval et al⁹³ studied clusters of ferroelectrically distorted KH_2PO_4 in the bulk 300 paraelectric solid.

Kolezynski and co-workers have used FP-LAPW DFT to study properties of a series of anhydrous oxalates^{94,95,96} particularly with respect to the behaviour of these salts under thermal decomposition.

3.2. Non-oxides

305 Here I shall cover mainly ionic solids and exclude those which could be regarded as alloy-like.

Yang et al⁹⁷ using DFT demonstrate a sequence of pressure-induced phase transitions in BaF_2 from fluorite to PbCl_2 to Ni_2In structures. Qiao et al have studied interstitial fluoride⁹ and Mg-doping⁹⁹ in LiBaF_3 . Kurzydowski et al¹⁰⁰ reproduced 310 the correct ferromagnetic semiconductor ground state of K_2AgF_4 using DFT calculations. Andriyevsky et al¹⁰¹ reported the first calculations of the electronic and optical properties of K_2ZnCl_4 in its ferroelectric phase.

Matar and Demazeau¹⁰² proposed the potential existence of a post-perovskite structure nitride, ThTaN_3 from their DFT calculations. Jha et al¹⁰³ used DFT to 315 predict phonon and thermodynamical properties of the antiperovskite structure solids AsNBa_3 and SbNBa_3 . Weng et al¹⁰⁴ have used DFT calculations to predict properties of a new class of Si-Ge oxynitrides, $\text{Si}_{1-x}\text{Ge}_x\text{N}_2\text{O}$, with potential for use as tunable dielectrics. Nakhil et al¹⁰⁵ used DFT calculations to obtain a plausible structural model of a proposed new tantalum oxide nitride, $\text{Ta}_3\text{O}_6\text{N}$.

320 Tan et al¹⁰⁶ obtained ground state properties and equations of state of ZnS

consistent with experiment and calculated vibrational contributions to thermodynamic properties. A DFT study of PtS by Marmier et al¹⁰⁷ has uncovered the existence of negative compressibility in this compound shortly before the pressure-induced phase transition from $P4_2/mmc$ to the less symmetric PdS structure (P4₂/m). Hamidani et al¹⁰⁸ have calculated structural and electronic properties of PdS₂ and PdSe₂. Bailey et al¹⁰⁹ used hybrid DFT to study defect formation in CuGaS₂ and found that this material is intrinsically p-type doped. Li et al¹¹⁰ have calculated electronic and optical properties of β -LaGaS₃. Extrinsic n-type doping is predicted to be impossible. Ouahrani et al¹¹¹ have calculated the properties of CdAl₂Se₄.

Maurya et al¹¹² showed, using FLAPW DFT calculations, that InN is more stable in the wurtzite phase than as a cubic close packed phase.

4. Zeolites and related structures

Two aspects of these solids are considered – structure and reactions within them.

I start with papers that consider rationalisation and prediction of structure. Zwijnenburg and Bromley¹¹³ used DFT calculations to show how varying the charge-compensating cation in aluminosilicates changes the order of stability of particular structures. They found that zeolite structures are favourable for large Group 1 cations. Pickard and Needs¹¹⁴ have studied chiral framework structures of the Group 14 elements C, Si Ge and Sn. Sastre and Corma¹¹⁵ considered zeolite structures made from germanate or silicogermanate gels and develop guidelines for the stability of germanium-containing zeolites, in particular that the presence of a double four ring was sufficient to stabilise a germanium-containing zeolite. Bushuev and Sastre¹¹⁶ considered guidelines for pure silica zeolites. These authors also considered occluded water and organic template molecules produced during zeolite synthesis¹¹⁷. Pongsai has used Monte Carlo and lattice statics methods to optimise the geometry of H-(Al)-ZSM-5. Grajciar et al¹¹⁸ have used DFT to investigate the effect of Al content on the properties of H-FER. Bushuev et al¹¹⁹ used atomistic simulations and molecular dynamics to investigate the role of water and hydroxyl groups in the synthesis of beta Zeolite polymorphs particularly BEC.

The next papers are concerned with properties of framework structures. Tielens and Dzwigaj¹²⁰ have used DFT calculations to probe acid-base sites in vanadium redox zeolites. Sastre et al¹²¹ have calculated OH stretching frequencies at various sites in mordenite and found a correlation with the electric field at the proton in the direction of the OH bond. Castro et al¹²² have used NMR CASTEP to assign ²⁷Al and ³¹P resonances in the molecular sieve AIPO4(SAT).

Finally I cover the interaction of molecules with zeolites. Gren et al¹²³ have used atomistic simulations to study the structure of siliceous and sodium aluminosilicate forms of Zeolite A surfaces and molecular dynamics of a slab of Zeolite A in water to investigate the interaction with water. Bordat et al¹²⁴ introduced a new force field for silicalite which maintains both framework flexibility and realistic electrostatic interactions with adsorbed water. Solans-Montfort et al¹²⁵ studied the interaction of hydrogen molecules with extraframework cations, Cu⁺ and FeO⁺ in chabazite. Danilczuk and Lund¹²⁶ used DFT to model the absorption sites for NO in Li⁺-exchanged Zeolite A. Liu et al¹²⁷ reported a DFT investigation of NO_x on silver-exchanged aluminophosphate molecular sieves. Zicovich-Wilson et al¹²⁸ have used hybrid DFT calculations to determine the mechanism of the elimination of F⁻ trapped

in the double four membered ring cages of octadecasil.

5. High T_c Superconductors

370 There is still interest in the cuprate superconductors but much effort is now directed
towards the more recently-discovered iron pnictide superconductors. Both classes
have in common a layer structure, the cuprates having layers of CuO and the iron
pnictide layers of FeX where X = S, Se, P, As. However these layers are different in
kind; the cuprate layers containing Cu as Cu(II) or Cu(III) and oxide ions and the
375 FeX layers containing formally low valence iron and being almost alloy-like.
Differences have also been noted in the superconducting mechanism.

Johnston et al¹²⁹ address the wide variety of T_c values in cuprate superconductors
and conclude that electron-phonon coupling plays a major role in determining T_c in
conjunction with some as yet unknown dominant mechanism. As one example, a
380 simplified model demonstrates that combining electron-phonon coupling with spin
fluctuations can increase T_c beyond the value due to electron-phonon coupling by
itself.

Wang et al¹³⁰ present ab initio calculations on β -pyrochlore superconductors
AOs₂O₆ with A = K, Rb, Cs.

385 A number of papers have used ab initio methods to study the band structure of Fe-
based superconductors, addressing such issues as the presence of Fermi surface
nesting, which has been connected to superconductivity. Nakamura's group have
performed DFT calculations on several iron pnictide superconductors. They find the
perovskite-based layer in Sr₂ScFePO₃ can give a good nesting condition^{131,132}. They
390 have also studied Sr₂VFeAsO₃¹³³, BaFe₂As₂, LiFeAs and FeSe¹³⁴ and compared low-
energy Hamiltonians for LaFePO, LaFeAsO, BaFe₂As₂, LiFeAs, FeSe and FeTe¹³⁵.
Johannes et al¹³⁶ considered the effect of doping and pressure on the magnetism and
lattice structure of BaFe₂As₂.

6. Nanostructures

395 Research on nanotubes and related structures still flourishes, but there is also now
considerable interest in the 2-D solid graphene. For example, Kvashnin et al¹³⁷ have
studied the mechanical properties of graphene membranes by molecular mechanics.
Two papers explore the difficult but important processes of obtaining graphene from
graphite. Boukhvalov and Katsnelson¹³⁸ showed, using DFT calculations, that the
400 uppermost layer of graphite when functionalised by phenyl groups becomes less
firmly bound and suggest it could be separated by mild sonication. Rasuli and Zad¹³⁹
used DFT to study the synthesis of graphene from graphite oxidation and
exfoliation.

Catlow et al¹⁴⁰ have reviewed the role of computational techniques for oxide and
405 sulfide nano-particles. Migani et al¹⁴¹ found a marked reduction in the energy of
oxygen vacancy formation for nanoparticles of ceria.

Work on nanotubes includes the Shokri and Khoeini¹⁴² investigation of the extent
of electron localisation in boron-doped superlattice carbon nanotubes as a function
of boron concentration, and a study by Zhang et al¹⁴³ of Al-doped silica nanotubes.
410 Hossain et al¹⁴⁴ obtained the band structure of anatase TiO₂ by DFT calculations and
predicted a possible band gap modification compared to the bulk solid.

Other structure-types have been studied. Zdzetis¹⁴⁵ used hybrid DFT to predict a

new family of Group 15 fullerenes. Li et al¹⁴⁶ explored the nature of the electronic states of direct band gap H-passivated silicon nanonets. Xu et al¹⁴⁷ have used DFT to study the effect on properties of N-doping in ZnO nanowires and Agrawal et al¹⁴⁸ used DFT to investigate failure in ZnO nanowires, comparing the results with previous interatomic potential calculations. Jiang et al¹⁴⁹ have used interatomic potentials in their study of the thermal conductivity of graphene nanoribbons. Shidpour et al¹⁵⁰ have used DFT to study the effect of sulfur vacancies in MoS₂ nanoribbons on the magnetic properties.

7. Applications in biology and earth science

Minerals are a rich area for computation as many are formed under conditions which are extremely hard to reproduce experimentally but can be modelled.

There have been a number of reports on minerals of biological interest such as calcite and hydroxyapatite. One aspect of biomineralisation is the use of inhibitors and/or promoters to obtain specific polymorphs or crystal shapes. Aschauer et al¹⁵¹ used molecular dynamics and atomistic simulation to investigate the effect on the growth of calcite crystals of polyacrylic acid and polyaspartic acid. Liu et al¹⁵² have studied adsorption of Ca on TiO₂ surfaces and concluded that their results offer a partial explanation for the formation of hydroxyapatite on alkali-treated Ti. Matos et al¹⁵³ used DFT calculations to investigate the stabilisation of Zn in hydroxyapatite. Zinc is an element naturally found as an impurity in biological hydroxyapatite (e.g. in bone) and plays an important role in the regulation of bone deposition and resorption.

Calcite is also an important mineral in earth science and there have been several studies in this context. Aurelio et al¹⁵⁴ have determined that Se can be incorporated into calcite by substituting for carbon. Ruiz-Hernandez et al¹⁵⁵ used atomistic simulations to study the incorporation of Sr into the calcium carbonate polymorph, aragonite.

Zhang and Wright¹⁵⁶ considered coupled substitution of H⁺ and Al³⁺ in forsterite (the Mg end olivine) where M = Al, Fe, Ga, Mn, Sc, Lu, Yb, Y, Gd, Eu, Nd and Pu. Caracas¹⁵⁷ reported studies on the perovskite to postperovskite phase transition in the Earth's lower mantle using the compounds AlFeO₃ and FeAlO₃. van Kan Parker et al¹⁵⁸ consider substitution mechanisms for trace element distribution between orthopyroxene and anhydrous silicate melt. Vinograd et al¹⁵⁹ used atomistic simulation to study solid solutions of diopside and K-jadeite. Gibbsite, Al₂(OH)₆ is a building unit of layered double hydroxides. Vyalikh et al¹⁶⁰ have used calculations to assign the ²⁷Al resonances in the NMR spectrum and hence identify two groups of structural OH groups - intralayer and interlayer in gibbsite. Driver et al¹³ used quantum Monte Carlo methods to investigate the equations of state of silica phases up to the core-mantle boundary of the Earth and predict a transition to the α -PbO₂ structure above the D" layer. The D" layer is the lowermost part of the Earth's mantle, adjacent to the core and has interesting seismic properties. As the pressure in this layer is around 135 GPa and the temperature about 4000 K it is difficult to synthesise possible components of this layer and measure their properties for evaluation against the seismic results.

The origin of water on Earth has been tackled by de Leeuw et al¹⁴ who found that adsorption of water onto interplanetary dust particles was viable.

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