s5.m16.o2 **Squeezing Magnets: Implications for Crystallography And Geophysics.** Gerd Steinle-Neumann, *Bayerisches Geoinstitut, University of Bayreuth, 95440 Bayreuth, Germany. E-mail: g.steinle-neumann@uni-bayreuth.de*

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Magnetism plays a central role in the understanding materials structure and behaviour, ranging from the stability of crystallographic phases to elastic properties. While in experimental measurements the magnetism is implicit and its importance can not readily be assessed, first principles computations based on density functional theory can access non-magnetic and magnetic candidate configurations and probe the influence of magnetic interactions on various physical properties. From such computations, for example, we understand that the ambient condition phase of iron, body centred cubic (bcc), is stabilized by the presence of magnetism [1]; similarly, the large thermal expansivity in face centred cubic (fcc) iron at high temperature is caused by magnetic interactions. Here I use first principles theory to examine magnetism in two important, prototypical, magnetic materials in the Earth sciences, pure iron and $Fe_3O_4$ magnetite. I probe the behaviour of magnetism as these materials are compressed, as well as its changing influence on physical parameters. For iron I will focus on predictions of an antiferromagnetic phase [2] in the high pressure polymorph, hexagonal close packed (hcp), and its resulting consequences on physical properties [3]. In magnetite the magnetic structure is determined by a complex interplay of the charges at the various Fe sites in the spinel structure that changes under pressure leading to coordination crossover within the structure [4]. Here I will show results from first principles theory that examine in detail this recently observed phenomenon of charge transfer in $Fe_3O_4$.

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s5.m16.o3 **Axial ratio and elastic constants of hcp Fe under Earth's core conditions.** C. M. S. Gannarelli[a], D. Alfè[a,b], M. J. Gillan[a], [a]*Department of Physics and Astronomy, University College London, Gower Street, London, WC1E 6BT, UK,* [b]*Research School of Geological and Geophysical Sciences, Birkbeck and University College London, Gower Street, London, WC1E 6BT, UK E-mail: CHE.GANNARELLI@UCL.AC.UK*

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A major controversy about the Earth's solid inner core concerns seismic anisotropy: the observation that seismic compression waves propagate approximately 3% faster along the polar axis than in the equatorial plane. The Earth's core is largely composed of Fe, with a solid inner and liquid outer core, and recent studies support the hypothesis that the phase of Fe in this region is hexagonal close packed (hcp). A simple model of the anisotropy has been proposed, based on partial alignment of hcp crystallites. A key ingredient of any such theory is single-crystal elastic constants $c_{11}$ and $c_{33}$.

The recent use of electronic structure theory to calculate Earth's core properties has had notable successes, including the use of molecular-dynamics and other approaches to address high-temperature properties[1, 2, 3]. Elastic constants in particular have been calculated at zero temperature[4], and also at high temperature using the particle-in-cell (PIC) approximation[5]. Significantly, the PIC approximation indicates a strong temperature dependence of the axial ratio *c/a*, leading to a strong temperature dependence of the elastic constants. This has the effect of reversing the crystallite orientation required to explain the observed seismic anisotropy. However, the usefulness of the PIC approximation remains controversial[6].

In order to help resolve this issue, we have performed *ab initio* electronic structure calculations of the axial ratio and elastic constants of hcp Fe at a range of pressures and temperatures relevant to the Earth's core. The calculations are based on density functional theory in the generalised gradient approximation, using techniques which have been highly effective in a range of previous work[7]. The statistical mechanical methods do not entail the approximations involved in the particle-in-cell model. Instead, we perform calculations in two stages. In the first stage we use *ab initio* calculations of the full phonon spectrum to obtain the free energy as a function of elastic distortion, and hence the equilibrium axial ratio and elastic constants as a function of temperature. In the second stage, we calculate the time-averaged stress as a function of distortion using *ab initio* molecular dynamics, to evaluate the size of anharmonic corrections.

Our harmonic calculations indicate that the variation with temperature of axial ratio is much weaker than suggested by previous calculations. Molecular dynamics calculations indicate in turn that anharmonic corrections are relatively small. We use our results to reassess the mechanisms of seismic anisotropy in the inner core.

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