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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