E1-49: Iron and its magnetic moment in metallic environments

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Rare-earth iron nitrides are emerging as an important class of magnetic materials. In certain rare-earth iron compounds, the insertion of nitrogen (boron etc.) has resulted in significant changes in magnetic properties in the form of higher Curie temperatures, enhanced magnetic moments and stronger anisotropies.

As a first attempt to understand some of the above, we have focussed on 2 nitride phases of *Fe*, namely Fe_4N (cubic) and $Fe_{16}N_2$ (tetragonal). These nitrides are fascinating examples of magnetic solids, with a mixture of bcc and fcc environments. The crystal structure of Fe_4N is a fcc lattice of *Fe* atoms with a nitrogen atom occupying the body centre position. There are 2 inequivalent *Fe* sites here, one being closer to nitrogen than the other. In $Fe_{16}N_2$ there are 3 inequivalent *Fe* sites, 2 of them closer to *N* than the other. $Fe_{16}N_2$ can be thought of as alternate units of fcc *Fe* and Fe_4N units, with the atoms allowed to relax. For the $Fe_{16}N_2$ phase, the average *Fe* moment reported by different experimental groups varies over a wide range of values, from 2.3 to 3.5 μ_B.