**First principles study on electronic properties of magnetite for spin polarized electron emission**

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Magnetite is a mineral and one of the main iron ores. With the chemical formula Fe3O4, it is one of the oxides of iron. Magnetite is the earliest discovered magnet, around 1500 B.C. It crystallizes in the inverse cubic spinel structure (Fd3m) above the so-called Verwey transition temperature which is about 120 K. It has been found that a high temperature phase magnetite has a negative polarization of 100% at the Fermi surface, i.e., near the Fermi surface, only the spin down subband exists and the spin-up subband is far away from the Fermi surface. As a half-metallic material, Fe3O4 shows normal metallic behavior in the minority spin, while at the same time there is a gap of about 0.5 eV in the majority spin at the Fermi level. Although extensive studies of magnetite with considerable effort have been carried out over the past decades, the interesting electronic, magnetic, and transport properties as well as the potential industrial applications in magnetic multilayer devices, magnetite has still attracted much attention in recent years. In this work, we study the electronic properties of magnetite using first principles or *ab initio* calculations based on density functional theory in order to investigate a spin polarized electron emission. The work functions of magnetite Fe3O4 on different surfaces have been determined. In addition, local work functions have been analyzed and the correspondences with electron charge density distribution have been found. With this approach, one can investigate spin polarized properties of different materials such as ferrite accurately and efficiently. The magnetite as a half-metal can possibly be used as a field emitter for generating a spin polarized electron emission which may help in future analysis of noninvasive surface probes for biological systems or nanoelectronics.

1. H. T. Jeng and G. Y. Guo, Phys. Rev. B **65**, 094429 (2002).
2. J. Noh, O. I. Osman, S. G. Aziz, P. Winget, and J.-L. Brédas, Chem. Mater. **27**, 5856-5867 (2015).
3. T. Pabisiak, M. J. Winiarski, T. Ossowski, and A. Kiejna, Phys. Chem. Chem. Phys. **18**, 18169 (2016).