First Principles Study on Electronic Properties of Magnetite for Spin Polarized Emission under an Electric Field

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Abstract- Magnetite is a mineral and one of the main iron ores. With the chemical formula Fe_3O_4, 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. In this work, we study the electronic properties of magnetite (100), (110), and (111) surfaces under external electric fields using first principles or *ab initio* calculations based on density functional theory. With an electric field applied, the surface properties could be modified. For example, the (111) surface with an O_2 termination, the half-metal behavior becomes metal behavior under a critical electric field. With a +U calculation, most of the surfaces with different terminations show half-metallic, different from those predicted by a without +U calculation. We can use an electric field to control the metallic properties to be metallic or half-metallic. Un addition, the effective work function changes under different field strength. By calculating the local work function, we can know the distribution of work function on a certain surface. The effective work functions of magnetite Fe_3O_4 on different surfaces have been determined. The local work function has been found to have the correspondences with the atoms' positions and charge densities. It is proposed that the magnetite as a half-metal can possibly be used as a spin-polarized electron source.

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