First-Principles Study of Magnetic Properties of ε-Fe_2O_3

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ε-Fe_2O_3 has been attracting strong attention as a novel magnetic material because of its largest coercivity, $H_C = 2$ T, among all of the oxides [1,2]. However, the origin of high coercivity remains unclear, which is crucial not only for scientific interests, but also for materials design. Also, the magnetization is so small due to superexchange interactions via oxygen atoms: its improvement is an important key for technological applications. In this study, we performed first-principles calculations on ε-Fe_2O_3, based on density functional theory. We show that the pristine ε-Fe_2O_3 exhibits zero magnetization, which is in contrast to the finite magnetizaion in experiments at low temperature [1]. The influence of a single oxygen vacancy is also discussed, where it is introduced in the unit cell with 40 atoms. It is clarified that only the introduction to a specific oxygen site contributes to finite magnetization, whose structure is the most stable among those having a single oxygen vacancy. In the presention, we also talk about the magnetic crystalline anisotropy, which is also strongly affected.

References:

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