Electronic phase transitions in thin magnetite films

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Abstract

Fe oxides are versatile materials present in a large number of applications from disparate fields, and in particular in emergent nanotechnologies related to environmental protection, bio-medicine or spintronics. Among them, magnetite (Fe_3O_4) occupies a relevant position. It is a half-metallic ferrimagnet with high magnetic moment and moderate conductivity, that undergoes a complex metal-insulator transition (the so-called Verwey transition) at low temperatures involving a structural transformation from the inverse spinel structure to a monoclinic symmetry, and the emergence of charge- and orbital-ordered patterns [1]. This transition is ultimately governed by electron-phonon couplings in the presence of strong electron correlations [2]. Interestingly, it has been shown that similar metal-insulator transitions can be induced by application of external electric fields in nanostructures, under hydrostatic pressure or strain, and at surfaces, eventhough much remains to be understood about the detailed microscopic characteristics of these induced transitions [3,4].

A large effort is currently devoted to the investigation of magnetite thin films. Magnetite-oxide heterostructures are currently under scrutiny for the design of novel devices that exploit magnetism, electron correlation effects and interface phenomena: spin valves controlled by charge-orbital order [5] or non-volatile resistance switching driven by ferroelastic strain [6] have been proposed. All these phenomena rely on the control of the properties of magnetite in thin film form. However, the effect of reduced dimensionality on the metal-insulator transition, and on the relative stability with respect to other Fe oxide phases with different stoichiometry, magnetism and conductivity is not clear.

Here we will address the study of thin magnetite films based on first-principles calculations. These calculations provide a unique tool to disentangle interface and bulk effects, and allow to simulate non-equilibrium conditions difficult to achieve in the experiments. We will focus on the effect of boundaries (both with the vacuum and with the substrate) and film thickness on the electronic and magnetic properties of different films. We will show how the emergence of charge and orbital order is intimately related to the symmetry of the film, and how it affects to magnetism and conductivity. Our results indicate the universality of the surface electronic gap, and its consequences on the existence of a threshold thickness to recover a Verwey-like transition. Finally, we will also provide a detailed description of the magnetic order and how it is much less affected by the thickness of the films. These results support the ability to exploit electronic transitions involving magnetic order in novel devices based on ultrathin magnetite films.

References

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Figures

Spin-resolved density of states of Fe in an ultrathin magnetite film compared to the bulk, showing tetrahedral (blue) and octahedral (black) sites.