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Electronic structure and electron spectroscopy of magnetic iron oxide nanoparticles J. GAZQUEZ, J. SALAFRANCA, Universidad Complutense de Madrid, Spain, M. VARELA, S. PENNYCOOK, Oak Ridge National Lab, S.T. PANTELIDES, Vanderbilt University, P. MORALES, ICMM-CSIC, Spain, N. PEREZ, A. LABARTA, X. BATLLE, Univ. Barcelona, Spain — Magnetic iron oxide nanoparticles are good candidates for biomedical applications due to their low toxicity and easy functionalization. We synthesized magnetite (Fe3O4) nanoparticles by a high temperature decomposition method. They present some very desirable properties for applications: very high saturation magnetization, and excellent degree of crystallinity. Transmission electron microscopy images, and electron energy loss spectroscopy with atomic resolution allow a composition map that shows small variations in relative composition between the core and the surface, and subtle changes in the absorption spectra. Our density functional (DFT) calculations address different factors contributing to the magnetic properties. Changes in the electronic structure correlate with different features in the experimental absorption spectra, yielding a better understanding of the magnetic order. We study the role of structural defects, the organic surfactant, stoichiometry and the nominal oxidation state of iron, and their effect in determining the equilibrium magnetic state. This work is supported by DOE Materials Sciences and Engineering Division and the European Research Council Starting Investigator Award.

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