Abstract Submitted
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Strong electron correlation on the Fe_3O_4(0 0 1) surfaces HENRY PINTO, Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 TKK, Finland, SIMON D. ELLIOTT, Tyndall National Institute, Lee Maltings, Cork, Ireland, ADAM FOSTER, R. M. NIEMINEN, Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 TKK, Finland — Magnetite Fe_3O_4 is a fascinating material that still is not well understood and presents challenges for the state-of-the-art computational methods. This transition metal oxide undergoes a first-order metal-insulator transition at T_V=120 K. The ferrimagnetic properties of Fe_3O_4 makes it a promising material for spintronic applications. We use a plane wave density functional theory in the generalized gradient approximation adding a Hubbard-U parameter to describe properly the strongly correlated Fe–3d electrons. Based on previous results [1], we compute the surface structure, magnetic properties and electronic structure of several Fe_3O_4(0 0 1) surfaces with $(\sqrt{2} \times \sqrt{2})R45^\circ$ reconstruction. The simulated scanning tunneling microscopy images of these surfaces are compared and discussed in the light of available experimental data. Finally, we analyze the possible existence of charge ordering on the Fe_3O_4(0 0 1) surface and the effect on the surface electronic structure with changing the value of the Hubbard-U parameter on the superficial Fe sites.

[1]H. Pinto, S. Elliott, J.Phys.: Condens. Matter **18**, 10427 (2006)

Henry Pinto
Laboratory of Physics, Helsinki University of Technology

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