Theoretical studies on strongly correlated systems: bulk and surfaces of magnetite Fe$_3$O$_4$ HENRY PINTO, SIMON ELLIOTT, NMRC, University College Cork — Transition metal oxides (TMOs) are important materials because of their wide range of properties, the underlying physics and the tremendous implications for tomorrow’s technology. Magnetite, Fe$_3$O$_4$ is one technologically important TMO that undergoes a first-order metal-insulator transition at $T_V = 120$ K as reported first by E. Verwey. We use density functional theory adding a Hubbard-U parameter (DFT+U) to account for intra-atomic interactions for the strongly correlated Fe:3$d$ electrons of Fe$_3$O$_4$. Applying plane-wave DFT within the generalized gradient approximation and appropriate parameters, we examine the electron-phonon effects that cause a small structural distortion and lead to the insulating state with low symmetry. The electronic structure for this phase presents a sub-band of partially-delocalised minority spin electrons below the Fermi level. Here we investigate the competing roles of the screened coulomb repulsion, Fe-O hybridization and Fe-Fe overlap. We also study the Fe$_3$O$_4$ (001) surface: $(\sqrt{2} \times \sqrt{2})R45^\circ$ slab is used and we consider both tetrahedral and octahedral terminations. The surface reconstruction, electronic structure, magnetic properties and surface energies are computed. The calculated superficial density of states of our optimal slab is compared with scanning tunneling microscope data. Finally we analyze the effect of the electron-phonon interaction in the electronic structure of the surface and the possible existence of charge ordering.

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Date submitted: 21 Mar 2013

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