Abstract Submitted
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Spectral and magnetic properties of hematite Fe2O3(001) surface: results from DFT+DMFT[1] ALAMGIR KABIR, VOLODYMYR TURKOWSKI, TALAT S. RAHMAN, Department of Physics, University of Central Florida — It has been demonstrated that strong correlation effects may significantly modify the spectrum of a system, in particular leading to an increase of the bandgap and to a change in the orbital occupancies, which affects the magnetic properties of the system. With this in mind, we have examined the spectral and magnetic properties of the hematite Fe2O3 film system with (001) surface orientation by using the combined density functional theory (DFT) and dynamical mean-field theory (DMFT) approach. We pay special attention to the surface geometry and electronic structure, magnetization and magnetic anisotropy (MA) of the system by performing calculations at different values of the parameters for the local Coulomb repulsion and exchange energy. To calculate the MA of the system, we propose and apply a combined Bruno model [1] within DMFT, and demonstrate that under-coordinated surface Fe atoms contribute significantly to the MA of the film. We also compare our results with the DFT+U solution [2] and show that the dynamical effects taken into account by the DMFT significantly affect system properties, notably leading to a decrease of the atomic magnetic moments. [1] P. Bruno, Phys. Rev. B 39, 865 (1989). [2] A. Kiejna and T. Pabisiak, J. Phys.: Cond. Mat. 24, 095003 (2012).

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