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**Role of non-local exchange in the electronic structure of correlated oxides** FEDERICO IORI, Universite Paris Sud - CNRS, MATTEO GATTI, Theoretical Spectroscopy Group LSI - CNRS Ecole Polytechnique Synchrotron SOLEIL, ANGEL RUBIO SECADES, Theory Department, Max Planck Institute for the Structure and Dynamics of Matter, Max Planck Society — Transition-metal oxides (TMO) with partially filled d or f shells are a prototype of correlated materials. They exhibit very interesting properties, like metal-insulator phase transitions (MIT) [1]. In this work we consider several TMO insulators in which Kohn-Sham LDA band structures are metallic: VO<sub>2</sub>, V<sub>2</sub>O<sub>3</sub>, Ti<sub>2</sub>O<sub>3</sub>, LaTiO<sub>3</sub> and YTiO<sub>3</sub>. In the past, this failure of LDA has been explained in terms of its inadequacy to capture the strong interactions taking place between correlated electrons. In the spirit of the Hubbard model, possible corrections to improve onsite correlation are the LDA+U [2] and LDA+DMFT [3] approaches. Here we make use of the HSE06 hybrid functional [4]. We show that, without invoking strong-correlation effects, the contribution of the non-local Fock exchange is essential to correct the LDA results, by curing its delocalization error. In fact, HSE06 provides insulating band structures and correctly describes the MIT in all the considered compounds [5]. We further discuss the advantages and the limitations of the HSE06 hybrid functional in correlated TMO [1] M. Imada et al., Rev. Mod. Phys. 70, 1039 (1998) [2] V.I. Anisimov, et al., Phys. Rev. B 44, 943 (1991). [3] A. Georges et al., Rev. Mod. Phys. 68, 13 (1996). [4] J. Heyd et al., J. Chem. Phys. 118, 8207 (2003); J. Heyd et al., J. Chem. Phys. , 219906(E) (2006). [5] F. Iori, M. Gatti, and A. Rubio Phys. Rev. B , 115129 (2012)

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