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Exchange an Correlation effects in the electronic properties of transition metal oxides: the example of NiO MATTEO GUZZO, LSI -ETSF, Ecole Polytechnique, France, MATTEO GATTI, Universidad del Pais Vasco, San Sebastian, Spain, LUCIA REINING — NiO, as a prototype for strongly-correlated materials, has been extensively studied experimentally and theoretically. Its Antiferromagnetic phase is reasonably well described in GW (a many-body approximated approach), but self-consistency is needed to obtain proper wavefunctions for the system. Still, agreement with experiment is not perfect. In particular, the unoccupied d-states result too high in energy by about 1 eV. In the present work we investigate the effects of vertex corrections derived from time-dependent density-functional theory on this result, starting from a simple LDA correction and going to more complex vertices including non-locality.

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