

Abstract Submitted  
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**DFT with larger supercells explains the band gap formation in the antiferromagnetic and paramagnetic phases of the Mott insulators MnO, FeO, CoO, and NiO**<sup>1</sup> ALEX ZUNGER, Renewable and Sustainable Energy Institute, University of Colorado, Boulder, GIANCARLO TRIMARCHI, Physics Dept., Northwestern U. — The existence of large band gaps both in the antiferromagnetic (AFM) and the paramagnetic (PM) phases of the classic Mott insulators MnO, FeO, CoO, and NiO has traditionally been discussed in terms of theoretical methods requiring both (i) simple (often primitive) unit cells and (ii) correlated-electron methodologies. We show that if condition (i) is avoided (by using supercells, such as PM special quasi-random structures, in which chemically identical atoms can have different local environments), then even without condition (ii) one can describe the gaps and moments within a single-determinant DFT band structure approach. In this approach gapping is caused by basic structure, magnetism, and bonding effects underlying DFT, not via dynamic correlation (absent from DFT). As long as correlation is simplistically considered as “anything that DFT does not get right”, gap formation in the AFM and PM phases is not due to correlation. This result defines the minimal theoretical methods needed to explain gapping and points to the possibility that some transition-metal oxides generally considered to have localized electrons detrimental to transport, could, in fact, rejoin the family of electronic semiconductors, to the benefit of a carrier transport technologies.

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