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Putting DFT to the Test: A First-Principles Study of Electronic, Magnetic, and Optical Properties of Co_3O_4 VIJAY SINGH, MONICA KOSA, KOUSHIK MAJHI, DAN THOMAS MAJOR, Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel, PROF. ARIE ZABAN COLLABORATION — First-principles density functional theory (DFT) and a many-body Green's function method have been employed to elucidate the electronic, magnetic, and photonic properties of a spinel compound, Co_3O_4. Co_3O_4 is believed to be a strongly correlated material, where the on-site Coulomb interaction (U) on Co d orbitals is presumably important, although this view has recently been contested. The suggested optical band gap for this material ranges from 0.8 to 2.0 eV, depending on the type of experiments and theoretical treatment. Thus, the correlated nature of the Co d orbitals in Co_3O_4 and the extent of the band gap are still under debate, raising questions regarding the ability of DFT to correctly treat the electronic structure in this material. To resolve the above controversies, we have employed a range of theoretical methods, including pure DFT, DFT+U, and a range-separated exchange–correlation functional (HSE06) as well as many-body Green's function theory (i.e., the GW method). We compare the electronic structure and band gap of Co_3O_4 with available photoemission spectroscopy and optical band gap data and confirm a direct band gap of ca. 0.8 eV. Furthermore, we have also studied the optical properties of Co_3O_4 by calculating the imaginary part of the dielectric function ($\mathrm{Im}(\varepsilon)$), facilitating direct comparison with the measured optical absorption spectra.

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