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Electronic structure of Cu_2O within GW approximation FABIEN BRUNEVAL, Ecole Polytechnique, CEA, CNRS, Palaiseau, NATHALIE VAST, LUCIA REINING — It is known that density functional theory fails to predict a gap in various insulating oxides like CuO. Cu_2O is a good starting point to address the fundamental issue of *3d* electrons of metals in oxides. This semiconductor material has indeed a cubic structure, a closed *d* shell, and is non-magnetic. We calculated its band structure within Density Functional Theory and GW approximation [1]. We studied the role of semicore states ($3s^2 3p^6$) and stated that their influence is slight on the Kohn-Sham band structure, but drastic on the GW one. Even a GW calculation including semicore states largely fails with the quasiparticle gap. Further approximations are usually used to perform a "standard" GW calculation. We extensively discuss the reliability of these technical approximations, and find that they perform well. The most dubious approximation is the equality between GW and LDA wavefunctions. Therefore, we obtained self-consistent quasiparticle wavefunctions within the static COHSEX approximation to the GW scheme. We show that subtle changes in the wavefunctions may have large effects on the different contributions to the band gap. [1] L. Hedin, Phys. Rev. **139**, A796 (1965).

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