# Electronic Excitations of $Cu_2O$ within GW Approximation

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Cuprous oxide has been extensively studied during the last decades, mainly because of its exciton series in the optical range. $Cu_2O$ is a good starting point to address the fundamental issue of transition metal oxides. Indeed, this material has a cubic structure, a closed $d$ shell, and is non-magnetic. The topic of transition metal oxides is now very important: it is known that density functional theory fails to predict a gap in various insulating oxides like CoO, CuO, $Ti_2O_3$.

We performed DFT and GW calculations using ABINIT package. We carefully studied the role of semicore states ($3s^2 3p^6$). Though deep in energy, these states have a large overlap with valence bands. Their influence is slight on the Kohn-Sham band structure. However, we state that the semicore states have to be included in the GW calculation to get meaningful results.

Even a GW calculation including semicore states largely underestimates the quasiparticle gap. Further approximations are used to conduct a "standard" GW calculation, as in ABINIT code: the use of a plasmon pole model, a first order perturbation scheme, etc.

We extensively discuss many of them and conclude that they are reliable. Then the failure of GW may lie in the neglect of vertex functions.