Electronic Excitations in CuO from a Many-Body Point of View
CLAUDIA RÖDL, FRANCESCO SOTTILE, LUCIA REINING, Laboratoire des Solides Irradiés, Ecole Polytechnique, 91128 Palaiseau cedex, France — The insulating transition-metal oxide CuO is considered a key to understanding the electronic structure of high-temperature superconducting cuprates, since it features similar bonding geometries. The photoemission spectra of this oxide, which is usually termed to be strongly correlated, have not been explained satisfactorily by first-principles calculations up to now. Special difficulties arise from the close entanglement of the structural and electronic degrees of freedom in this compound, which is due to the unoccupied Cu 3d orbitals. In contrast to the local-density approximation of density-functional theory (DFT), which predicts CuO to be a metal, we obtain finite band gaps by means of hybrid functionals containing screened exchange and the DFT+U method. Starting from these qualitatively correct band structures, we perform many-body calculations in the GW approximation. The various approaches to the one-particle excitation spectra are compared to experimental results. We discuss whether or not the peaks occurring in the photoemission data are quasiparticle excitations or satellite structures, respectively.