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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.

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