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**First principles study of electronic and structural properties of CuO** BURAK HIMMETOGLU, MATTEO COCCIONI, University of Minnesota — The ground state of CuO is particularly challenging to study with DFT-based computational techniques even below its Neel temperature. This situation is due to the inability of most approximate DFT energy functionals to describe electronic regimes that are dominated by many-body effects. In this study, we show how a description of the ground state of this material in better agreement with observations can be obtained using extended Hubbard-based corrective energy functionals (DFT+U and DFT+U+V). In particular we uncover an orbitally ordered insulating ground state for the cubic phase of CuO (that was expected, but never reported before) whose appearance is determined by a fine interplay between correlation effects and magnetic interactions. Starting from this ground state we also study the tetrahedral distortion of the unit cell (recently reported in experiments), characterizing the reorganization of the electronic states and identifying all the equilibrium structures.

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