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Electronic properties of copper aluminate examined by three theoretical approaches NIELS CHRISTENSEN, Aarhus University, AXEL SVANE, Aarhus University, Aarhus, Denmark — Electronic properties of 3R.$CuAlO_2$ are derived vs. pressure from ab initio band structure calculations within the local-density approximation (LDA), LDA+U scheme as well as the quasiparticle self-consistent GW approximation (QSGW, van Schilfgaarde, Kotani, and Falaev). The LDA underestimates the gap and places the Cu-3d states at too high energies. An effective U value, 8.2 eV, can be selected so that LDA+U lowers the 3d states to match XPS data and such that the lowest gap agrees rather well with optical absorption experiments. The electrical field gradient (EFG) on Cu is in error when calculated within the LDA. The agreement with experiment can be improved by LDA+U, but a larger U, 13.5 eV, is needed for full adjustment. QSGW yields correct Cu-EFG and, when electron-hole correlations are included, also correct band gaps. The QSGW and LDA band gap deformation potential values differ significantly.

Niels Christensen
Aarhus University

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