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Ground-state properties of the three-band Hubbard model[1] SHIWEI ZHANG, ETTORE VITALI, ADAM CHICIAK, HAO SHI, College of William and Mary — The three-band Hubbard model proposed by Emery describes the CuO_2 plane in cuprate superconductors by retaining both Cu and O orbitals in a minimal sense. Applying the latest developments in the auxiliary-field quantum Monte Carlo (AFQMC) method, we investigate ground-state properties of this model at half-filling and when lightly (under-)doped. The AFQMC uses generalized Hartree-Fock (GHF) trial wave functions to control the sign problem. A self-consistent constraint [2] is applied. We also determine the unrestricted Hartree-Fock (UHF) and GHF ground states and compare their predictions with those from AFQMC. Similarities and differences between the three-band model and one-band Hubbard model will be discussed.

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[2]M. Qin, H. Shi, S. Zhang, arXiv:1608.07154 (2016).

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