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Magnetic spiral induced by strong correlations in MnAu<sub>2</sub> JAMES GLASBRENNER, NRC/NRL, KONRAD BUSSMANN, IGOR MAZIN, NRL — The compound MnAu<sub>2</sub> is one of the oldest known spin-spiral materials, yet the nature of the spiral state is still not clear. The spiral cannot be explained via relativistic effects due to the short pitch of the spiral and the weakness of the spin-orbit interaction in Mn, and another common mechanism, nesting, is ruled out as direct calculations show no features at the relevant wave vector. We propose that the spiral state is induced by a competition between the short-range antiferromagnetic exchange and a long-range interaction induced by the polarization of Au bands, similar to double exchange. We find that, contrary to earlier reports, the ground state in standard density functional theory is ferromagnetic, *i.e.*, the latter interaction dominates. However, an accounting for Coulomb correlations via a Hubbard U suppresses the Schrieffer-Wolff type s - d magnetic interaction between Mn and Au faster than the superexchange interaction, favoring a spin-spiral state. For realistic values of U the resulting spiral wave vector is in close agreement with experiment.

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