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Collapse and control of the $MnAu_2$ spin spiral state through pressure and dopin JAMES GLASBRENNER, National Research Council/Naval Research Lab — $MnAu_2$ is a spin spiral material with ferromagnetic Mn layers that rotate from plane to plane. The spiral angle θ decreases with pressure and collapses to a ferromagnetic state above a critical threshold, although different experiments do not agree on whether the collapse is first or second order. To resolve this contradiction, we employ density functional theory to calculate magnetic energies in the spiral state under both pressure and charge doping and fit the results to the $J_1-J_2-J_3-J_4$ Heisenberg model, which predicts either first or second order phase transitions depending on the set of exchange parameters. At ambient pressure, $MnAu_2$ sits very close to a dividing line separating first and second order transitions, and applying either pressure or electron doping shifts the system towards the second order region of parameter space. Our findings show how variations in material quality can impact how the spiral state collapses, which resolves the contradiction in pressure experiments. Our results also suggest that $MnAu_2$ is amenable to engineering via chemical doping and to controlling θ using pressure and gate voltages, which holds potential for integration in spintronic devices.

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