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Spin-orbit correlated magnetic order in honeycomb α-$RuCl_3$ VIJAY SHANKAR VENKATARAMAN, HEUNG-SIK KIM, HAE-YOUNG KEE, University of Toronto — There has been a lot of recent interest in the combined effects of spin-orbit coupling (SOC) and electronic correlations in transition metal compounds. $RuCl_3$ with layered honeycomb structure was proposed as a candidate material, where SOC boosts the electronic interaction, leading to an insulating phase. However, the role of SOC is not clear in materials with 4d-orbitals, since SOC strength is weaker than 5d-orbital materials. Here we study electronic band structures of honeycomb $RuCl_3$ using ab-initio and tight binding methods, and estimate its SOC strength. We find that SOC in $RuCl_3$ is not strong enough to justify an effective $j_{eff} = 1/2$ single band unlike in the iridates. However, when electronic interactions are introduced, a magnetic order develops, and upper- and lower-Hubbard bands are characterized by $j_{eff} = 1/2$ and $3/2$, respectively. Within a mean field theory with multi-orbital bands, we find that a zig-zag magnetic order is a ground state. Experimental implications are also discussed.

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