Competition between spin-orbit coupling and magnetic exchange splitting in Ca_2RuO_4

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The layered perovskite Ca_2RuO_4 has attracted considerable interest owing to its complicated electronic structures. Ca_2RuO_4 is antiferromagnetic insulating below 110 K, and paramagnetic insulating from 110 K to 357 K. Under external pressure, Ca2RuO4 undergoes an antiferromagnetic-ferromagnetic transition at 0.5 GPa. Surprisingly, the observed ferromagnetic moment M=0.4 μ_B/Ru is much smaller than the expected value of 2 μ_B/Ru. In this work, the magnetic properties of Ca_2RuO_4 are investigated by using the density functional calculations including the spin-orbit coupling and Coulomb repulsion. It is found that the low moment state originates in a Coulomb-enhanced spin-orbit splitting, which strongly suppresses the spin-moment. A simple formula is provided to discuss the competition between the spin-orbit coupling and magnetic exchange splitting. The electronic structures of Ca2RuO4, including the antiferromagnetic insulating, paramagnetic insulating, and ferromagnetic metallic, can be consistently explained within this competitive picture.