Competition between spin-orbit coupling and magnetic exchange splitting in Ca$_2$RuO$_4$

Guo-Qiang Liu
Ningbo Institute of Material Technology and Engineering,
Chinese Academy of Sciences, Ningbo 315201, China

The layered perovskite Ca$_2$RuO$_4$ has attracted considerable interest owing to its complicated electronic structures. Ca$_2$RuO$_4$ is antiferromagnetic insulating below 110 K, and paramagnetic insulating from 110 K to 357 K. Under external pressure, Ca$_2$RuO$_4$ undergoes an antiferromagnetic-ferromagnetic transition at 0.5 GPa. Surprisingly, the observed ferromagnetic moment M=$0.4 \mu_B$/Ru is much smaller than the expected value of $2 \mu_B$/Ru. In this work, the magnetic properties of Ca$_2$RuO$_4$ 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 Ca$_2$RuO$_4$, including the antiferromagnetic insulating, paramagnetic insulating, and ferromagnetic metallic, can be consistently explained within this competitive picture.