

La₂Co₂Se₂O₃: A Quasi-two-dimensional Mott insulator with Unusual Co Spin State and Possible Orbital Ordering

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SUPPORTING INFORMATION PARAGRAPH

Supplementary Band-structure Calculation Result

In the main article, the density of states (DOS) of Co atoms in $\text{La}_2\text{Co}_2\text{Se}_2\text{O}_3$ were shown and discussed in details. Here we present supplementary plots of density of states (DOS) versus energy, as shown in figure S1. The total DOS clearly indicates a band gap of ~ 1.5 eV. No spin polarization is evident, consistent with the antiferromagnetic ground state. In the projected DOS for the oxygen within Co_2O planes, there exists a strong orbital polarization for the valence electrons near Fermi level. By contrast, the projected DOS for Se $4p$ has no such orbital polarization.

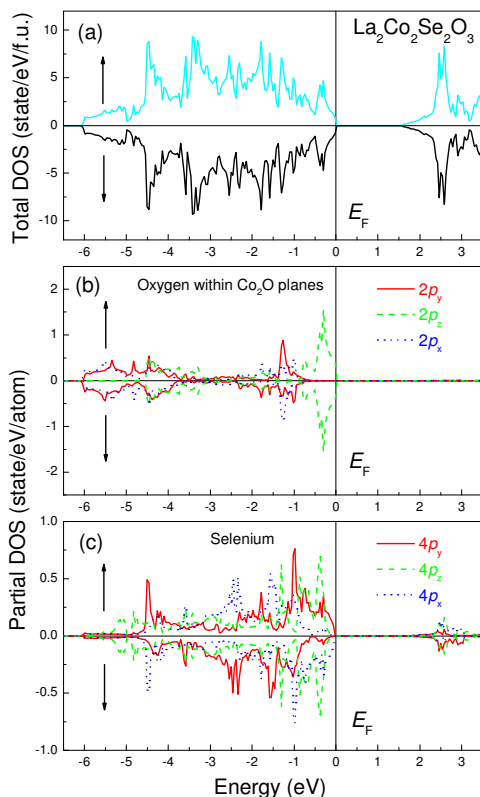


Figure S1. Supplementary plots of density of states (DOS) versus energy for $\text{La}_2\text{Co}_2\text{Se}_2\text{O}_3$ from LSDA+ U calculations. (a) total DOS; (b) projected DOS for the oxygen within Co_2O planes; (c) projected DOS for the selenium atoms.