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Electronic Structure and Bulk Spin Valve Behavior in $Ca_3Ru_2O_7$

DAVID SINGH, Oak Ridge National Laboratory, SUSHIL AULUCK, IIT Roorkee, India — The perovskite based ruthenates show a remarkable range of electronic and magnetic properties, even though they are all based on Ru^{4+} ions in octahedral environments with corner sharing bonding topologies. These behaviors include robust itinerant ferromagnetism, paramagnetic bad metal properties, unconventional superconductivity, Mott insulating properties and metamagnetic quantum critical behavior. The bilayer, so- called 327 compounds are of particular interest because of their borderline properties. We report density functional calculations of the magnetic properties and Fermiology of $Ca_3Ru_2O_7$. The ground state consists of ferromagnetic bilayers, stacked antiferromagnetically. The bilayers are almost but not exactly half-metallic. In the ferromagnetic state opposite spin polarizations are found for in-plane and out-of-plane transport. Relatively high out of plane conductivity is found for the majority spin, which is relatively weakly conductive in- plane. In the ground state in-plane quantities are essentially the same, but the out of plane transport is strongly reduced. This work was supported by the Department of Energy.

David Singh

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