

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Magnetic ordering and structural transition in layered Li_2RuO_3 ¹

DEVINA PILLAY, MICHELLE JOHANNES, Naval Research Laboratory — Li_2RuO_3 is a layered, triangular-lattice metal oxide system much like Na_xCoO_2 , NaNiO_2 and LiNiO_2 with the exception that one of every three transition metal ions (Ru) is replaced by a Li ion. This results in a honeycomb arrangement of spin-carrying ions and eliminates the magnetic frustration intrinsic to the triangular lattice. Here we investigate the electronic structure of Li_2RuO_3 , especially in relation to its magnetic ordering both in-plane and between adjacent planes. We find that the dimerization of Ru atoms within the metal-oxide planes acts in conjunction with magnetic ordering to establish a gapped, magnetic ground state. The change in the energy level spectrum brought on by the formation of spin-polarized Ru-Ru molecular orbitals replaces the expected Jahn-Teller mechanism as a way of relieving a degeneracy at the Fermi energy.

¹Funded by the Office of Naval Research. DP is funded by the National Research Council.

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Date submitted: 03 Dec 2007

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