Magnetic ordering and structural transition in layered Li$_2$RuO$_3$\textsuperscript{1}

DEVINA PILLAY, MICHELLE JOHANNES, Naval Research Laboratory — Li$_2$RuO$_3$ is a layered, triangular-lattice metal oxide system much like Na$_2$CoO$_2$, 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$_2$RuO$_3$, 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.

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