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Molecular orbitals vs. relativistic orbitals in t_{2g} honeycomb lattices: SrRu_2O_6 as compared to Na_2IrO_3 , RuCl_3 , and Li_2RuO_3 .¹ IGOR MAZIN, Naval Research Laboratory, SERGEY STRELTSOV, Institute of Metal Physics, Ekaterinburg, Russia, KATERYNA FOYEVTSEVA, University of British Columbia, Canada — t_{2g} states on a honeycomb lattice tend to form non-dispersive localized states even if large intersite hopping is present. In the nonrelativistic case, these are molecular orbitals (MO) localized on metal hexagons, if the ligand-assisted nearest and next nearest neighbor hoppings, t'_1 and t'_2 , dominate, or dimers (DO), if the direct overlap, t_1 , dominates. In the ultrarelativistic limit t_{2g} form effective relativistic orbitals (RO), $j_{eff} = 3/2$, which are atomically localized if t'_1 is the dominant hopping. On the first glance, the three regimes are defined by the conditions $t'_1 \gg t_1, \lambda$ or $t_1 \gg t'_1, \lambda$ or $\lambda \gg t_1, t'_1$. In reality, the latter condition is never fulfilled, especially in ruthenates, yet not only Na_2IrO_3 , but also RuCl_3 appear to be in a regime dominated by RO, even though the residual effect of MO critically influences magnetic interactions, while Li_2RuO_3 , not far removed from RuCl_3 in the parameter space, is firmly in the DO regime. Most surprisingly, SrRu_2O_6 , which is even closer to RuCl_3 , happens to be fully in the MO regime, with negligible spin-orbit effects. In this talk, we will show that an additional, decisive factor is the doping level per site. The principal difference between Na_2IrO_3 or RuCl_3 , Li_2RuO_3 , and SrRu_2O_6 is that the first two have one t_{2g} hole per site, the second one two holes, and the last three electrons. In particular, the total dominance of MO in the latter compound fully explains its unique and unexpected magnetic properties.

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