# 3D electronic structure in the potential Kitaev Quantum Spin Liquid, α-$RuI_3$

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Quantum Spin Liquids are an exciting class of material with localized and entangled spin 1/2 electronic states, with great interest for quantum computing application. Among them the Kitaev QSL are characterized by a honeycomb lattice showing no magnetic order at very low temperature. In general, the promising family of compounds are the magnetically frustrated quasi-2D systems. The well-known α-$RuCl_3$ is a Mott insulator with a zig-zag antiferromagnetic transition [1]. Recently, single crystals of a cousin material, α-$RuI_3$ has been synthetized. In this isostructural compound no long-range magnetic ordering was found down to at least 0.35 K [2].

In this study we investigate the 3D band structure of α-$RuI_3$ measured by micro-ARPES with a spatial resolution of 4 μm. The high symmetry cuts (fig. 1) show clear evidence of metallic states and significant broadening of the bands at higher binding energies attributed to the strong electron correlations. The bulk Fermi Surface is characterized by an electron pocket dispersing around the GA axis and 6-hole pockets at the edge of the BZ. Our DFT calculation with SOC and $k_z$ broadening agree reasonably well with the measurements. The "spiral" features of the Fermi Surface are a direct consequence of the reduced symmetry of the R-3 phase of α-$RuI_3$. The detailed photon energy dependence study shows a strong $k_z$ variation indicating that the interlayer stacking order plays a key role in the electronic structure of the α-$RuI_3$.

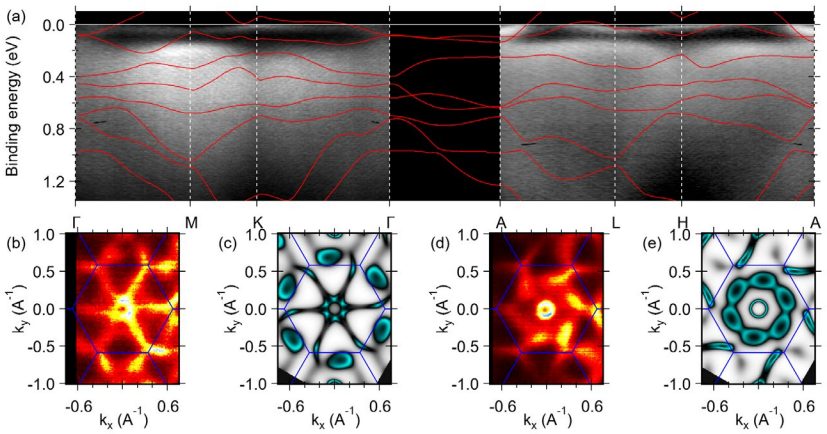


**Fig. 1.** (a) Experimental band dispersion of RuI3 along ΓMKΓALHA path. The red lines are DFT with SO band dispersion (b) and (d) Experimental Fermi surfaces at $k_z$=0 and c*/2 respectively. The blue hexagon is the simplified Brillouin zone. (c) and (e) Fermi surfaces extracted from DFT with $k_z$ broadening at $k_z$=0 and c*/2 respectively.

**References**

[1] Sears, J. A. et al. Magnetic order in α-RuCl3: a honeycomb-lattice quantum magnet with strong spin-orbit coupling. Phys. Rev. B 91, 144420–144424 (2015)

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