Highlights

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Hallmarks of Hunds coupling in the Mott insulator Ca_2RuO_4

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A paradigmatic case of multi-band Mott physics including spin-orbit and Hund's coupling is realized in Ca_2RuO_4. Progress in understanding the nature of this Mott insulating phase has been impeded by the lack of knowledge about the low-energy electronic structure. We provide, using angle-resolved photoemission electron spectroscopy, the band structure of the paramagnetic insulating phase of Ca_2RuO_4 and show how it features several distinct energy scales. Comparison to a simple analysis of atomic multiplets provides a quantitative estimate of the Hund's coupling J=0.4 eV. The experimental spectra are in agreement with electronic structure calculations performed with Dynamical Mean-Field Theory. The crystal field stabilization of the d_{xy} orbital due to c-axis contraction is shown to be essential to explain the insulating phase. These results underscore the importance of multi-band physics, Coulomb interaction and Hund's coupling that together generate the Mott insulating state of Ca_2RuO_4.

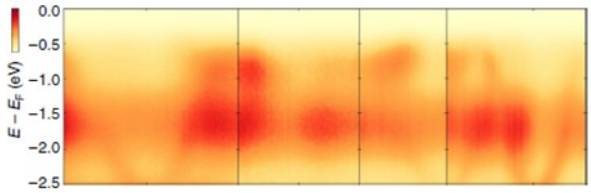

Fig.1: ARPES spectra recorded along high-symmetry directions with 65 eV circularly polarized light.

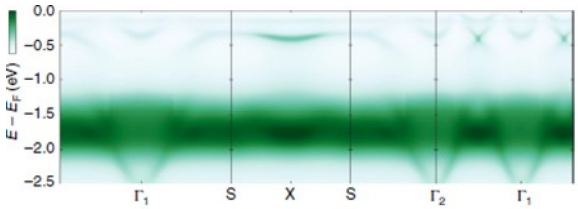

Fig.2: DMFT calculation of the spectral function, with Coulomb interaction U=2.3 eV and a Hund's coupling J=0.4 eV. Dark colours correspond to high intensities.