Disentangling the contribution of e_g and t_{2g} orbitals to the exchange and Coulomb correlation effects in the FM/AFM magnetic exchange coupling by Angle Resolved APECS (Auger-photoelectron coincidence spectroscopy)

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The mutual Coulomb interaction of valence electrons in solids causes deviation from the independent particle behavior, and become relevant in narrow band systems and whenever the dimensions are reduced to the nanoscale. Nowadays DFT is the main computational tool to compute electronic structure of systems of realistic complexity. In spite of its undoubted successes there are still difficulties to properly account for correlation driven effects such as magnetism.

The two hole final state of Core Valence Valence Auger decays, is used as two electron correlation spectroscopy of valence band. In angle resolved – Auger photoelectron coincidence spectroscopy (AR-APECS), the angle resolved time coincidence detection of the Auger electron together with its parent photoelectron allows to catch information on both the two holes left behind, in a way that parallel and anti-parallel spin hole pairs can be selected. This allows to probe the effective correlation energy U_{eff}, for different multiplet final states [1], as well as for different spin combinations in the final state [2].

A ferro\antiferromagnetic bilayer (Fe/CoO) was used to highlight the role of electron correlation in the exchange-coupling at the interface. U_{eff} has been experimentally determined for any possible combination of orbital (e_g or t_{2g}) and spin (majority or minority) pairs of the valence electrons and, for the first time, Coulomb and exchange contribution to the correlation energy have been singled out [3].

Thin magnetic films have shown a sizable variation of the exchange-correlation energy as their thickness reduces to a few monolayers. The disappearance of the AR-APECS dichroism in thin films for temperatures just above the critical thresholds [4] indicates a collapse of the surface magnetic order at the atomic level, presumably due to a strongly reduced exchange field in the surface compared to that in the bulk.

References

[1] R. Gotter et al., Phys.Rev.B **79**, 075108 (2009).
[2] R. Gotter et al., Phys.Rev.Lett. **109**, 126401 (2012)
[3] R. Gotter et al., Phys.Rev.Lett. **125**, 067202 (2020); M. Sbroscia et al., JMMM **589**, 167872 (2021)
[4] R. Gotter et al., EuroPhys.Lett. **96**, 37008 (2011); R. Gotter et al., Phyis.Rev.B **88**, 094403 (2013).