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## Localized or delocalized K-holes in N<sub>2</sub>: Photoelectron-Auger electron coincidence experiments with high energy resolution

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**Synopsis :** For K-shell ionization of N<sub>2</sub> photoelectron auger electron coincident angular distributions show that pathways with *gerade* and *ungerade* K-hole state can interfere. On the other hand high resolution photoelectron spectroscopy seems to indicate that the *gerade* and *ungerade* hole state can be separated in energy. The present experiment aims to combine the high energy resolution with full angular detection of Auger and Photoelectron to resolve this seeming contradiction.

The debate around the localization or delocalization of a K-shell hole induced by x-ray photon ionization in N<sub>2</sub> or O<sub>2</sub> puzzled scientist for a long time. In 2008 M. Schöffler *et al.* [1] gave a well-detailed picture resolving the apparent contradiction of the two views. Using an Auger electron detection in coincidence with the photoelectron, the symmetry breaking (localization) or preservation (delocalization) of the molecule seems to depend on how the entangled Auger electron is detected. This interpretation however assumed that the pathway including a *gerade* or *ungerade* K-hole state can perfectly interfere. This is in seeming contradiction to the known energy splitting of about 100meV between the 1σ *ungerade* and 1σ *gerade* state and raises the question how two pathways can interfere, which can at least partly be separated in the photoelectron energy.

The reaction mechanism consists in the absorption of one photon to ionize the molecule, followed by the emission of an Auger electron and the consequent fragmentation in two N<sup>+</sup> ions. The orbital

from where the photoelectron is ejected from, could be either a coherent or an incoherent superimposition of the 1σ *ungerade* and 1σ *gerade* molecular orbitals. Due to the entangle state between the Auger probe and the induced photoelectron, angular distribution patterns look different in the two cases.

The present study tries to fully and precisely resolve the intermediate quantum mechanical state of K-shell holes in energy in addition to measuring the molecular frame angular distribution of both electrons in coincidence. The detection setup is a custom modified and optimized COLTRIM system aiming for sub 100meV electron energy resolution. The experiment is performed at beamline P04 PETRA III facility providing a sub 100meV energy resolution at unprecedented photon flux. First results will be presented at the meeting.

### References

- [1] M. Schöffler *et al.*, Science, Vol. 320. no. 5878, pp. 920 - 923 (2008).

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