INTERNSHIP and THESIS PROPOSAL

Orbital Imaging in Correlated Fermions Materials

(A thesis grant is already obtained and available to start as soon as desired)

Materials with strong correlations exhibit a diverse range of physical phenomena, such as unconventional superconductivity, heavy fermion behavior, metal-insulator transitions, exotic magnetism such as quantum spin liquid, multiferroicity. Typically composed of transition-metal, rare-earth, or actinide elements, the atomic-like d or f orbitals are the key component to create these exciting phenomena. The complex interplay between band formation, local correlation, and atomic multiplet effects results in numerous phases nearly degenerate in energy, allowing for highly tunable material properties through doping, temperature, pressure, or magnetic field variations. Understanding the behavior of d and f electrons is crucial, requiring the identification of orbitals actively involved in ground state and low-energy excitations. Currently, these orbitals are mainly inferred from optical, x-ray, and neutron spectroscopies, where spectra analysis relies on theory or modeling. However, this poses a challenge as ab-initio calculations usually face limitations due to the many-body nature of the problem. Recently, a novel experimental approach was proposed to yield a direct imaging of the atomic orbitals at play in materials from spectroscopic measurements [1–3]. The technique relies on non-resonant inelastic x-ray scattering (IXS), also known as X-ray Raman Scattering (XRS), performed at high momentum transfer with intense synchrotron light. Owing to this methodology, a visual representation of the active orbital can be obtained, possibly helping to discern the actual structure of the relevant atomic orbitals in a crystal (see Fig. 1), which can be confronted to calculations of the electronic structure eventually.

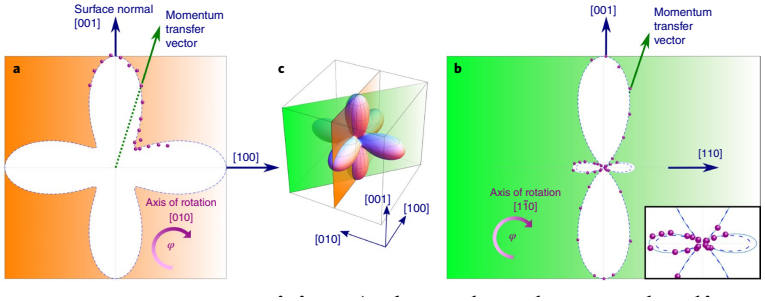

Fig. 1 : XRS integrated intensities of M1 (3s → 3d) edge spectra plotted on the projections of the orbital shape of the $3d_{x2-y2}$ and $3d_{z2}$ hole density (from Ref. [1]) in NiO single crystal.

Lately, our team has succeeded in developing this technique at Synchrotron SOLEIL, acquiring expertise in data measurement and analysis. As a result, we have imaged relevant orbitals in different compounds of recent interest such a $BaCoS_2$, $BaNiS_2$, V_2O_3 or CuO. This PhD project aims to take this new approach to address several of the most challenging topics in quantum materials, namely :

- Quantum molecular magnets, whose occupied orbitals, responsible for magnetism, change depending on pressure [4], requiring instrumental development.
- Metal-Insulator transitions in vanadates (VO2, V2O3) under temperature and pressure [4-6].
- Unconventional one-dimensional superconductors with orbital order in superconducting compounds [7] .

Possibility to performe state of the art DMFT calculation to corroborate the results are possible in collaboration with Benjamin Lenz (IMPMC, Sorbonne Université

[1] H. Yavaş, et al. Nat. Phys. 15, 559 (2019) [2] B. Leedahl et al. Nat. Commun. 10, 5447 (2019) [3] A. Amorese et al. Phys. Rev. X 11, 011002 (2021) [4] G. J. Halder et al. Angew. Chem., Int. Ed., 50 , 419 (2011) [5] Balédent V et al. High Pressure Research 36, 371 (2016) [6] Arcangeletti E et al. Phys Rev Lett. 2007 ;98 :196406. [7] Mitrano M et al. Phys Rev B. 2012 ;85 :184108. [8] Hosoi S et al. Phys. Rev. Research 2, 043293 (2020)

Contacts :
Victor Balédent victor.baledent@universite-paris-saclay.fr https://equipes2.lps.u-psud.fr/victor-baledent
Jean-Pascal Rueff jean-pascal.rueff@synchrotron-soleil.fr
Location: Laboratoire de Physique des Solides (UMR8502) and SOLEIL synchrotron