THESIS PROPOSAL

Laboratory name: LPS (UMR8502) and IMPMC (UMR 7590)
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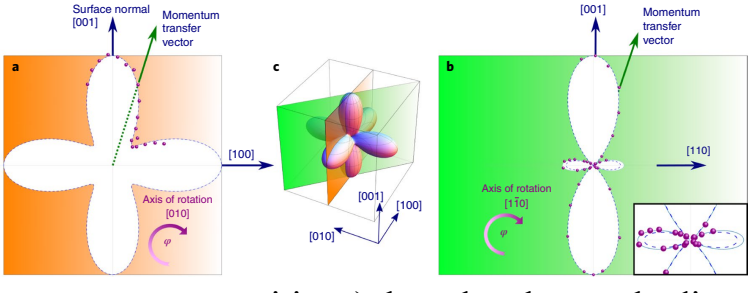
Internship location: Laboratoire de Physique des Solides and IMPMC

Orbital Imaging in Correlated Fermions Materials

A recent spectroscopic technique reported in March 2019 enables the direct imaging of orbitals. The measurement is based on Non-resonant Inelastic X-ray Scattering (NIXS) by observing some low-energy absorption resonance in the energy loss spectrum (incident minus final energy). The method has been successfully applied in NiO with a $3d^8$ electronic configuration, revealing the d_{z2} and d_{x2-y2} orbitals of the *3d* holes of Ni atoms (see figure from Nature Physics 15, 559 (2019)). This new kind of imaging opens up a wide and completely new field of investigations, in particular for strongly correlated electrons materials where small changes of electronic structure generate remarkable properties (heavy fermions, superconductors, Mott insulators etc…)



In this internship/thesis, we propose to use this technique to study different materials where the orbital shape and orientation is central to understand their remarkable properties. In particular, we would like to extend this technique to low temperature and high pressure, something that has not been done so far. This would open a wide range of possibilities for a large number of condensed matter thematics. Sample characterization and preparation, together with data analysis will be performed at LPS, experiences will be performed at GALAXIES beamline at SOLEIL and possibly other synchrotrons in Europe. We already have good quality data on CuO crystals that need to be analyzed and interpreted in light of DMFT calculation. For this reason, a significant part of the internship/thesis will concern DMFT calculation at IMPMC.

Another project focuses on the reorientation of orbitals under pressure in systems with molecular magnetism ($CuF_2(H_2O)_2(pyz)$). Under pressure, the orbital carrying the magnetism passes successively through the 3 possible planes in a narrow pressure range (P<4 GPa). This challenging project has been submitted to the SOLEIL synchrotron, which if accepted, will take place during the internship period (May-July).

In summary, this thesis project combines state-of-the-art theoretical and experimental techniques (DMFT, NIXS), in order to establish a new way of observing the electronic and magnetic properties of materials, while developing the possibilities in terms of sample environment (temperature, pressure, electric/magnetic field...).