INTERNSHIP PROPOSAL

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Internship location: Sorbonne Université, 4 place Jussieu, 75005 Paris

Thesis possibility after internship: YES
Funding: YES/NO (PhD scholarship from ED-PIF or ANR funding)

Correlations meet core-level spectroscopies: Calculating Non-resonant Inelastic X-ray Spectra from first principles

Summary:
Determining which wave functions contribute to the ground state formation of the solid is key to determining electronic and optic properties of quantum materials. However, few experimental techniques allow to directly measure the orbital composition of the ground state, in particular for strongly correlated materials with partially filled d shells. A novel experimental technique, non-resonant inelastic x-ray scattering (NIXS), promises exactly that: Imaging the orbitals in quantum materials directly in real-space[1].

Here, we propose to calculate the NIXS cross section of a transition metal oxide, CuO, based on state-of-the art many-body simulations. We will use a combination of *ab initio* density functional theory and dynamical mean-field theory[2] to describe the electronic structure of the material. The latter is well suited to incorporate electron-electron interactions needed to treat strongly correlated electron systems. Building on a recently developed cluster solver, we will calculate in a second step the NIXS cross section[3], which amounts at the M_1-edge to a quadrupolar transition from the core 3s-shell to the valence 3d-shell of copper.

This Master thesis will pursue the development of a computational scheme to simulate a very timely spectroscopic technique. By comparing to NIXS measurements done by our collaborators, we will study the orbital composition of the material's ground state as a function of temperature. The internship is part of a project on methodological developments to calculate core-level spectra for correlated materials, which can be further pursued in form of a thesis.

[1] *Nat. Phys.* **25**, 559 (2019); [2] *Rev. Mod. Phys.* **78**, 865 (2006); [3] *Phys. Rev. Lett.* **99**, 257401 (2007)

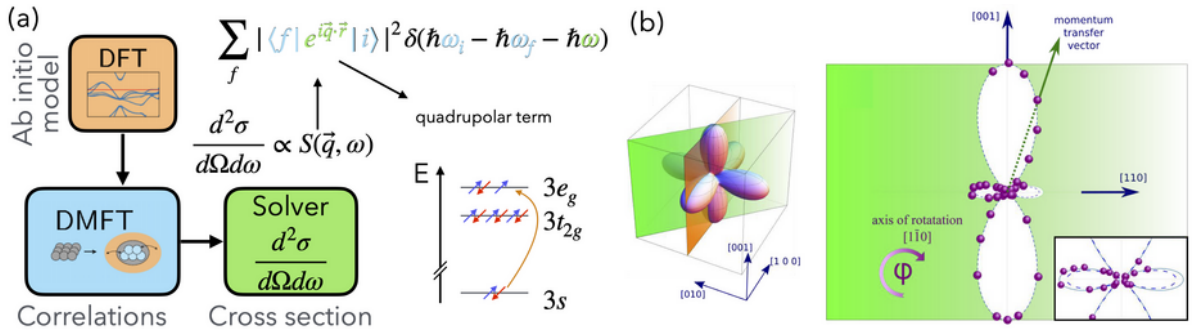

Figure 1: (a) Workflow of the NIXS calculation including DFT+DMFT to calculate the NIXS cross section at the M-edge. (b) Measured orbital shape of the 3d(3z2-r2) hole density in NiO. Figure taken from Ref. [1].

Condensed Matter Physics: YES Soft Matter and Biological Physics: NO
Quantum Physics: MAYBE Theoretical Physics: YES