SCIENCES SORBONNE UNIVERSITÉ

2021-2022

Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22
Director: A. Marco Saitta

Title: Electron Energy Loss Spectra from Quantum Cluster Techniques

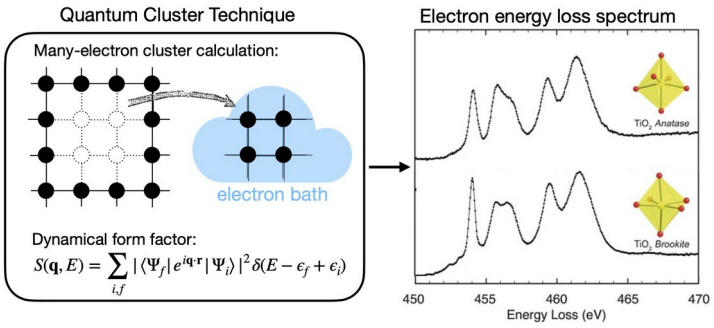
Keywords: Solid state physics, theoretical spectroscopy, quantum cluster techniques, correlated materials

Scientific description:

Electron Energy Loss Spectroscopy (EELS) is a versatile technique to probe a wide range of material's properties, ranging from low-energy vibrational to optical or plasmonic excitations. At large energy losses, core-shell ionisations can be observed, bringing insight into the electronic structure of a material down to the atomic scale[1].

Here, we will calculate EELS spectra by means of a multi-layered approach consisting of *ab initio* density functional theory, which is used to describe the electronic structure of the material, and quantum cluster techniques, which are well suited to incorporate electron-electron interactions needed to treat strongly correlated electron systems[2]. Building on a novel quantum cluster solver, we will use Green's function based techniques such as the variational cluster approximation and the cluster dynamical impurity approximation to calculate core loss spectra of selected benchmark materials.

This Master thesis will pursue the application of a recently developed quantum cluster code to the calculation of EELS spectra. By comparing to actual EELS measurements, the student will study the effect of cluster size and geometry on the spectral features of the core loss spectrum.



[1] G. Radtke and G. A. Botton. "Energy loss near-edge structures." *Scanning Transmission Electron Microscopy*. Springer (2011), p. 207-245. ; [2] B. Lenz et al, J. Phys.: Condens. Matter **31** 293001 (2019).

Techniques/methods in use: Quantum cluster techniques, Density functional theory
Applicant skills: Solid background in condensed matter physics; motivation for theoretical physics; basic programming skills (C++ or python)
Industrial partnership: N

Internship supervisors:

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Guillaume RADTKE, guillaume.radtke@upmc.fr, 01 44 27 50 63

Internship location: Sorbonne University, IMPMC lab, campus Pierre et Marie Curie

Possibility for a Doctoral thesis: Yes (to be discussed with the applicant)