INTERNSHIP PROPOSAL

Laboratory name: Institut de minéralogie, de physique des matériaux et de cosmochimie (IMPMC), Sorbonne Université – CNRS – MNHN
CNRS identification code: UMR 7590
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Web page: https://impmc.sorbonne-universite.fr/en/research_teams/quantum-theory-of-matter.html
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)

Strong Correlations in Ruby: New Methods for an Old Problem

Summary:
When light travels through a ruby, yellow-green and violet radiations are absorbed, while red and some blue are transmitted, giving the mineral its characteristic colour. This phenomenon is largely related to electronic excitations occurring within the *3d*-shell of Cr^{3+} impurities in the Al_2O_3 matrix. X-ray absorption spectroscopy at the Cr-L_{23} edge is a very direct experimental, element-selective probe of these *3d* states and has been extensively employed over the last decades to understand the electronic properties of ruby[1,2]. Unfortunately, due to the complexity of this material involving strongly correlated *3d* electrons, the modelling of these spectroscopic signatures has mostly relied on semi-empirical approaches, giving an approximative and misleading picture of its underlying many-body physics.

The recent development of very efficient numerical schemes for dealing with strongly correlated electronic systems offers, however, new opportunities to gain insight into the physics of ruby[3]. The objective of this master thesis is to use state-of-the-art techniques to calculate XAS signatures in ruby entirely from first-principles (see Figure 1) based on density functional theory (DFT), Wannier functions and constrained Random Phase Approximation (cRPA)[4]. 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] E. Gaudry *et al. Phys. Chem. Minerals* **32** (2006) 710 ; [2] M. Hunault *et al. J. Phys. Chem. A* 122 (2018) 4399;
[3] H. Saito *et al. Phys. Rev. B* **108** (2023) 035141; [4] K. Nakamura *et al. Comput. Phys. Comm.* **261** (2021) 107781.

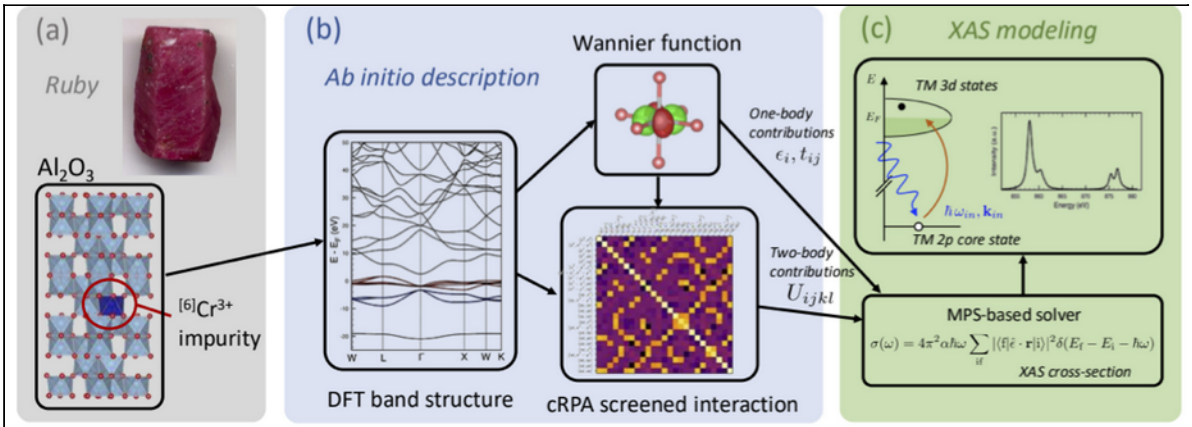

Figure 1: (a) Atomic structure of ruby; (b) Workflow of the ab initio determination of the local model parameters (c) XAS probe of the local, orbital and element selective Cr-3d states.

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