SCIENCES SORBONNE UNIVERSITÉ

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Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
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Title: Deciphering niobium crystallographic environment in ore minerals through first-principles calculations of X-ray absorption spectra

Keywords: X-ray absorption spectroscopy, First-principles calculations, Crystallography, Niobium, Ore mineralogy

Scientific description:
Niobium (Nb) is a transition metal with unique properties including a high melting point, corrosion resistance and superconductivity properties making it valuable for a wide range of applications. However, Nb deposits are scarce, making it a "critical" element. Diversification of sourcing and improved exploitation require an in-depth understanding of the processes concentrating niobium. These processes depends on its chemical form in the environment which can be determined through X-ray absorption spectroscopy. So far, the knowledge on Nb X-ray spectroscopic properties is limited due to the scarcity of the studies focusing on this element. The objective of this work is to expand our theoretical understanding of the relationship between Nb crystallographic environment and X-ray absorption spectral features, a condition to develop our understanding of Nb chemistry and mineralogy.
In this frame, Nb *K*-edge X-ray absorption spectra will be acquired on a set of Nb-bearing minerals representative of the ore mineralogy existing in major deposits, in particular in iron and titanium oxide. The local Nb environment in these oxides remains unknown. Density functional theory-based relaxation of the atomic positions in a supercell of Nb-substituted oxides followed by a self-consistent field calculation can unravel this environment. Subsequent computation of X-ray absorption spectra will confirm the validity of these first-principles calculations and give the possibility to decipher the origin of the spectral features in terms of Nb local environment. These results will be key to the development of Nb-based industrial products and to unravel the processes concentrating Nb in major geological deposits.

Techniques/methods in use: Density functional theory-based calculations, Synchrotron-based X-ray absorption spectroscopy experiments
Applicant skills: programming, basic skills in crystallography and density functional theory approaches
Industrial partnership: N

Internship supervisor(s) (name, email, phone, webmail): Mathieu Chassé (mathieu.chasse@sorbonne-universite.fr, 01 44 27 41 13) / Delphine Cabaret
Internship location: IMPMC, Sorbonne Université
Possibility for a Doctoral thesis: Y, to be discussed with the applicant