



A Grenoble, au centre des Alpes, le LETI est un institut de recherche appliquée en micro et nano technologies, technologies de l'information et de la santé. Interface privilégiée du monde industriel et de la recherche académique, il assure chaque année le développement et le transfert de technologies innovantes dans des secteurs variés via des programmes de recherche utilisant nos plateformes technologiques.

Research topics: Solid state physics, quantum chemistry

Influence of local atomic structure on XPS spectrum using ab initio calculations

Context :

X-ray Photoelectron Spectroscopy (XPS) is a useful and common experimental tool to characterize the chemical composition of materials by detecting the energy level of electron core states. Recent XPS experiments performed at CEA-Leti show that the electron core levels in an alloy material with dopant are shifted systematically with the doping concentration and the alloy mixing ratio. Such a fact suggests that XPS experiments may give more information on the local atomic structure other than the standard chemical composition.

Work description:

In this internship, you will explore the structural dependence of the XPS spectra using ab initio methods, such as density functional theory (DFT) and many-body perturbation theory (GW). Besides theoretical simulations, you have access to experimental results for comparison and interact with experts in XPS.

Laboratoire d'accueil: LETI/DCOS/SCME/LSM

Adresse:

17 avenue des martyrs
38054 GRENOBLE Cedex 9

Contacts :

Dr. Benoit Sklénard (Benoit.SKLENARD@cea.fr)

Dr. Jing Li (Jing.LI@cea.fr)

Formation Requisite: M2

Durée: 6 months

Date démarrage: February 2021

Possibilité de thèse: oui