SCIENCES SORBONNE UNIVERSITÉ

2024-2025

Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

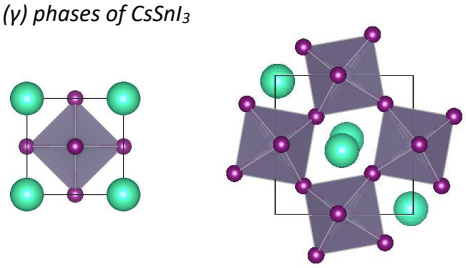
Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22

Title: **Predicting the band gap of a non-toxic metal halide perovskite for solar cell applications**

Keywords: ab initio simulations, electronic structure, phase transitions, many-body theory, photovoltaics

Scientific description:
Inorganic metal halide perovskites are promising materials for future efficient and low-cost solar cells. The band gap depends on the composition and one of the most interesting candidates is cesium lead iodide that combines good electronic properties (e.g. band gap of 1.7 eV) with improved stability. The drawback is that lead is toxic, and, hence, it is desirable to replace it with an element like tin. In this project, we will investigate the influence of this substitution on the electronic structure. The band gap is expected to reduce, and, similarly to the lead-based materials, various phase transitions occur as a function of temperature. While experiments show a weak variation of the band gap across the phase transitions, ab initio calculations predict a gap variation as large as 0.5 eV. The difference is expected to originate in thermal fluctuations (not taken into account in standard band gap calculations), but a complete understanding is missing. Taking into account many-body effects and spin-orbit coupling we will determine the band structure of the high- and low-temperature phases and analyse the origin of the discrepancies. We will also investigate whether it is possible to induce a topological transition by applying hydrostatic pressure.

High-temperature (α) and room-temperature (γ) phases of $CsSnI_3$



Techniques/methods in use: Many-body theory (GW), Electronic structure calculations (VASP, Wein2K, Exciting)
Applicant skills: Background in solid-state or chemical physics. Interest in theory and simulations. Programming skills in Python are necessary.
Industrial partnership: N
Internship supervisor(s):
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Internship location: Institut de Minéralogie, Physique des Matériaux et Cosmochimie (IMPMC), Equipe: TQM: https://impmc.sorbonne-universite.fr/fr/equipes/theorie_quantique_des_materiaux.html
Possibility for a Doctoral thesis: Y