SCIENCES SORBONNE UNIVERSITÉ

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Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

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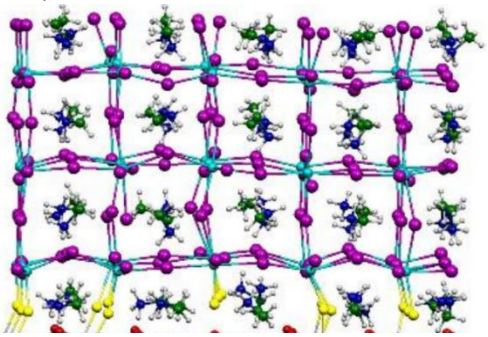
Title: *Ab initio* atomistic study of organic-inorganic perovskites phase diagrams

Keywords: Ab initio simulations, electronic structure, perovskites

Scientific description:

Organic-inorganic perovskites offer a rich opportunity to develop future devices for photon-electron conversion due to their cheap fabrication process from liquid solution, their low crystallization temperature, and their excellent optoelectronic properties. In this project, developed within an experimental collaboration with Nanyang Technical University in Singapore, we aim in the long term at studying the nucleation and growth of organic-inorganic perovskite based on the observation of the nucleation and growth processes at nanometer scale and ab initio atomistic simulations. In a similar way, we aim at calculating the thermodynamically favored atomistic pathways leading amorphous perovskites into their crystalline forms, as a function of the external parameters mentioned above.



The results of the simulations will first be used to draw the phase diagrams versus the temperature for the MAPbI3 and FAPbI3 systems. The influence of the solvent and anti-solvent will also be mapped in a multi-dimensional phase diagram. Based on these findings, more complex systems will be studied in the longer term, such as the triple-cation perovskite systems (AxByC1-x-y)(Pb(IzBr1-z)3 where A, B and C are the cations for various I/Br ratios (z). The final simulation step will be toward Ruddlesden–Popper layered perovskites. The phase diagrams and the synthesis routes predicted from the simulations will guide the project toward more stable and defect-free structures and possibly to the discovery of new organic-inorganic perovskite phases.

Techniques/methods in use: Density Functional Theory, *ab initio* molecular dynamics
Applicant skills: strong background in solid state and statistical physics, propensity for simulations and/or programming
Industrial partnership: N
Internship supervisor(s) (name, email, phone, webmail):
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Internship location: IMPMC – Campus Pierre et Marie Curie – T 2324
Possibility for a Doctoral thesis: Y (specific funding likely, otherwise doctoral school)