

**A post-doc position in the area of the computational condensed-matter physics,
in link with society goal of “Decarbonized energy supply”**

Laboratoire des Solides Irradiés, Ecole Polytechnique, IPP

**Theoretical study of photoexcited carrier dynamics and exciton-phonon interaction in
hybrid perovskites**

Photoexcited carrier dynamics in hybrid perovskites currently attracts attention because of the potential photovoltaic and optoelectronic applications of these materials [1]. From a more fundamental perspective, photoexcited carrier relaxation in hybrid perovskites involves complex phenomena such as exciton-phonon and polaron-phonon interactions [2,3], which present a challenge from experimental and theoretical points of view, and are subject of intense scientific activity. At LSI, photoexcited carrier dynamics in hybrid perovskites is currently studied with time-resolved spectroscopy (tr-ARPES). Recently, the formation of Wannier excitons in two-dimensional hybrid perovskite $(\text{BA})_2(\text{MA})_2\text{Pb}_3\text{I}_{10}$ was demonstrated by tr-ARPES and DFT band structure calculations [4]. Further understanding of the carrier dynamics requires the study of exciton-phonon interactions, in order take into account exciton screening by phonons [3,4] as well as to describe the carrier dynamics in real time.

This is the reason why we propose this post-doc project, which aims to develop the DFT-based description of the exciton-phonon interaction and dynamics in hybrid perovskites, in link with experiments by FEMTOARPES team of LSI and with beyond-DFT band structure calculations in collaboration with V. Gorelov. The developments will be done in the framework of density functional perturbation theory (DFPT) and time-dependent Boltzmann transport equations which allows to describe the electron (hole)-phonon coupling and carrier relaxation dynamics in numerous materials, the domain of expertise of TSM team of LSI [5]. Also, this project aims to establish a collaboration with the team of Prof. M. Calandra in University of Trento, who have recently developed a novel theoretical approach to describe nonequilibrium photocarrier and phonon dynamics, which allows to include the effects of carrier-carrier, carrier-phonon, and phonon-phonon scattering into the relaxation dynamics description [6]. This approach, based on DFT and DFPT, allows also to include many-body perturbation theory, in order to describe excitons, exciton-phonon interactions and exciton screening by phonons. Applying this technique to a challenging $(\text{BA})_2(\text{MA})_2\text{Pb}_3\text{I}_{10}$ to understand the carrier dynamics is the main goal of the project. Once this approach is developed, we aim to apply it to perovskites which are of interest to our partner IPVF institute, for example to double halide perovskites [8].

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For further information about the project, please contact: Jelena Sjakste: jelena.sjakste@polytechnique.edu