INTERNSHIP PROGRAM FOR INTERNATIONAL STUDENTS

INTERNSHIP SUBJECT FORM

Name of the Host Laboratory	Laboratoire des Solides Irradies
Website of the Host Laboratory	https://portail.polytechnique.edu/lsi/en
Research Group	Materials Science Theory: https://portail.polytechnique.edu/lsi/en/research/materials-science-theory
Internship Supervisor	Jelena Sjakste
Internship Subject	Hot electron relaxation in layered quasi-2D semiconductors: ab initio theoretical study
Student's level	☐ Advanced Undergraduate Students (3rd or 4th year) ☒ Master's students (1st or 2nd year) ☒ PhD students
Proposed Duration	☐ 3 months ☒ 4 months ☒ 5 months ☒ 6 months
Prerequisites	The proposed internship subject requires an understanding of quantum mecanics and solid state physics. It will involve theoretical as well as computational work, so some ability and willingness to program is essential. Some experience in computers with linux operating system is a plus, as well as some notions in Fortran. Previous experience in density functional theory is a plus, but is not mandatory.
Internship description (max. 15 lines)	Interaction of excited electrons with lattice vibrations (phonons) plays a central role in nanoelectonics, for optoelectronic devices, photovoltaic and thermoelectric materials [1,2]. Recently, we developed an approach which allows to describe hot-electron relaxation dynamics and to interpret time- energy- and angle-resolved photoemission experiments in layered semiconductors potentially promising for optoelectronics [1,2], as well as in 3D bulk materials (Si, GaAs). During this internship, we propose to study, using the methods based on Density Functional Theory, the atomic structure, the electronic and vibrational properties, and the electron-phonon coupling coefficients and hot electron relaxation dynamics in a 3D and quasi-2D semiconductors. The work will be performed in close link with ongoing experiments. [1] Z. Chen, C. Giorgetti, J. Sjakste, R. Cabouat, V. Véniard, Z. Zhang, A. Taleb-Ibrahimi, E. Papalazarou, M. Marsi, A. Shukla, J. Peretti, L. Perfetti, *Ultrafast electron dynamics reveal the high potential of InSe for hot-carrier optoelectronics,* Phys. Rev. B **97**, 241201(R) (2018). [2] J. Sjakste, K.Tanimura, G. Barbarino, L. Perfetti, N. Vast, *Hot electron relaxation dynamics in semiconductors: assessing the strength of the electron–phonon coupling from the theoretical and experimental viewpoints,* J. of Phys.: Cond. Mat, 30, 53001 (2018).