INTERNSHIP PROGRAM FOR INTERNATIONAL STUDENTS

INTERNSHIP SUBJECT FORM

Name of the Host Laboratory	Laboratoire des Solides Irradiés
Website of the Host Laboratory	https://portail.polytechnique.edu/lsi/en https://portail.polytechnique.edu/lsi/en/research/materials-science-theory
Research Group	Materials Science Theory
Internship Supervisor	Nathalie VAST
Internship Subject	Modelling electronic density fluctuations with time-dependent density functional theory
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 mechanics and solid state physics. It will involve theoretical and/or computational work: some ability and willingness to programming is essential. Some knowledge in computers with linux operating system and/or basis in the Fortran programming language and/or previous experience in density functional theory are a plus.
Internship description (max. 15 lines)	The signature of plasmons in electron energy loss (EEL) spectra of noble metals and their surfaces shows the richness of the physics underlying the various contributions to the density fluctuation in these materials [1], and their modelling – through the computation of the inverse of the frequency-dependent dielectric tensor - has become tractable nowadays within time density functional perturbation theory (TDDFPT). The present internship work will be devoted to the modelling of electronic density fluctuations within TDDFPT in some bulk material and eventually, it time allows it, its surfaces, with the code turboEELS in the Quantum ESPRESSO suite of softwares [2]. [1] *Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method* Oleksandr Motornyi, Nathalie Vast, Iurii Timrov, Oscar Baseggio, Stefano Baroni, and Andrea Dal Corso, Phys. Rev. B 102, 035156 (2020). [2] *Advanced capabilities for materials modelling with Quantum ESPRESSO*, P. Giannozzi et al., J. Phys.: Condens. Matter 29, 46590 (2017). http://iopscience.iop.org/article/10.1088/1361-648X/aa8f79/meta

The boxes marked with cross implies eligible