



INTERNSHIP PROGRAM FOR INTERNATIONAL STUDENTS

INTERNSHIP SUBJECT FORM

Name of the Host Laboratory	LSI
Website of the Host Laboratory	https://portail.polytechnique.edu/lsi/en/research/materials-science-theory
Research Group	TSM Material Science Theory
Internship Supervisor	Nathalie VAST
Internship Subject	Modelling boron carbides with density functional theory
Student's level	<input type="checkbox"/> Advanced Undergraduate Students (3 rd or 4 th year) <input checked="" type="checkbox"/> Master's students (1 st or 2 nd year) <input checked="" type="checkbox"/> PhD students
Proposed Duration	<input type="checkbox"/> 3 months <input checked="" type="checkbox"/> 4 months <input checked="" type="checkbox"/> 5 months <input checked="" type="checkbox"/> 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, 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)	<p>Boron carbide is expected to be used as the neutron absorber for future reactors of generation IV. It is a material in which the disorder induced by point defects is crucial. The modelling on the quantum scale of its physical properties is therefore challenging, as se a large number of atoms is required. Nonetheless, the LSI-TSM group has proposed atomic models accounting for the stabilization of boron carbide.</p> <p>In the present internship, we propose to progress in the validation of the atomic models of boron carbide with the calculation of two kinds of theoretical spectroscopy: Raman spectroscopy, requiring phonon calculations; and nuclear magnetic resonance calculations, requiring the computation of NMR the ¹³C chemical shielding. Results will be compared to experiments. The method will be density functional perturbation theory as implemented in the Quantum Espresso package. Calculations will be performed in the framework of a EU PRACE Research Infrastructure.</p> <p>A. Jay, O. Hardouin Duparc, J. Sjakste, and N. Vast, <i>Theoretical phase diagram of boron carbide from ambient to h pressure and temperature</i>, J. Appl. Phys. 125, 185902 (2019). https://doi.org/10.1063/1.5091000 Editor's pick</p>