



INTERNSHIP PROGRAM FOR INTERNATIONAL STUDENTS

INTERNSHIP SUBJECT FORM

Name of the Host Laboratory	Laboratoire de Chimie Moléculaire (LCM)
Website of the Host Laboratory	https://portail.polytechnique.edu/lcm/en
Research Group	
Internship Supervisor	Gilles FRISON
Internship Subject	Computational chemistry applied to homogeneous catalysis
Student's level	<input checked="" 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 checked="" type="checkbox"/> 3 months <input checked="" type="checkbox"/> 4 months <input checked="" type="checkbox"/> 5 months <input checked="" type="checkbox"/> 6 months
Prerequisites	knowledge in Molecular Chemistry and strong interest in Theoretical/Computational Chemistry
Internship description (max. 15 lines)	<p>State-of-the-art quantum chemistry tools (DFT, NBO, topological approach, energy decomposition analysis) will be used to study a challenging problem in homogeneous organic or organometallic catalysis. This problem will be related to the design of catalyst with the desired electronic structure, the prediction of region- and stereoselectivities or the exploration of reaction mechanism. These subjects are studied theoretically in our group in strong collaboration with experimentalists.</p>