**INTERNATIONAL PROGRAM FOR INTERNATIONAL STUDENTS**

**INTERNATIONAL SUBJECT FORM**

<table>
<thead>
<tr>
<th>Name of the Host Laboratory</th>
<th>Laboratoire de Chimie Moléculaire (LCM)</th>
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<tbody>
<tr>
<td>Website of the Host Laboratory</td>
<td><a href="https://portail.polytechnique.edu/lcm/en">https://portail.polytechnique.edu/lcm/en</a></td>
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<td>Research Group</td>
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<td>Internship Supervisor</td>
<td>Gilles FRISON</td>
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<td>Internship Subject</td>
<td>Computational chemistry applied to homogeneous catalysis</td>
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**Student's level**
- x Advanced Undergraduate Students (3rd or 4th year)
- x Master's students (1st or 2nd year)
- x PhD students

**Proposed Duration**
- x 3 months
- x 4 months
- x 5 months
- x 6 months

**Prerequisites**
Knowledge in Molecular Chemistry and strong interest in Theoretical/Computational Chemistry

**Internship description (max. 15 lines)**
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.