

The objective of the present project is to study the tribochemistry of selected compounds suggested by the Total company. The candidate will perform in silico tests based on molecular dynamics to study the chemical reactions occurring under load and shear.

Both computational chemistry and experimental investigations will be conducted simultaneously. A collaboration with an experimental group at the Ecole Central de Lyon is envisaged based on the use of the gas phase lubrication equipment that allows to perform the tribological test in the presence of selected molecules in the environment and identify the products of the reactions by means of in situ XPS analysis.

The aim of the project is to provide understanding on such experiments by means of molecular simulations.