The objective of the present project is to study the effects of H_2O, H_2 and O_2 molecules on the tribological properties of two solids in contact. The candidate will perform in silico tests based on ab initio molecular dynamics to study the chemical reactions occurring under load and shear.

The simulations will highlight both the reaction kinetics and the effects of surface passivation on the friction coefficient. Energy barriers will also be calculated by means of the nudged elastic band method.

The wear process due to atom-by-atom removal will also be investigated by means of static calculations in the presence of a tensile stress.