During the course of a chemical reaction, reactants need to overcome an energy barrier to transform into products. The energy for this process is typically provided by heat or light. A fundamentally different way of initiating or accelerating a reaction is the use of mechanical forces. Understanding reaction kinetics in the presence mechanical forces represents a fascinating fundamental problem with important applications in different fields, such as tribochemistry, where chemical reactions involving lubricant or environmental molecules are activated at the interface between two solids in relative motion.

The aim of the present research activity is to develop and apply advanced computational techniques to design materials to reduce friction. By advancing tribological materials impressive energy savings, and consequent reduction of CO_2 emissions, can be obtained. However, optimizing lubricant materials is challenging because their performances are ruled by molecular-level processes that occur at the buried interface, which are extremely difficult to monitor by experiments. Simulations can play a decisive role here, in particular those based on quantum mechanics, which is essential to accurately describe the reactions in conditions of enhanced reactivity as those imposed by the mechanical stresses applied.