

## **Abstract for the general public in English**

The ultimate goal of lubrication is reducing energy consumption with obvious advantages in terms of profitability and, even more important, in reducing greenhouse gases in Earth's atmosphere. Well-known applications include bearing, shafts, blades, slitters, gears, pistons, chains and several components in the automotive, aerospace and marine industry. Traditionally, lubrication is performed using oily and fat liquids, which unavoidably leads to serious environmental problems such as the disposal of used substances. Furthermore, liquid lubricants have no use at low temperatures and low pressures demanded e.g. for space applications. It is thus of primary importance to develop alternative lubrication techniques avoiding the use of liquids and, before testing them, to characterize and possibly understand their functioning under model conditions such as repeated scratching of the lubricated surface by means of indenters with well-defined geometries.

This OPUS project aims to investigate atomic-scale wear mechanisms of transition metal dichalcogenides (TMD) in crystalline and amorphous forms as well as of monolayers of the same materials on silicon wafers. TMDs are ultimately intended to be used as solid lubricants or protective coatings for machine elements, but the project will not develop out of specific engineering problems. A strong emphasis will be rather put on understanding the complex relations between the friction force variations recorded during wear tests and the morphology of the nanostructures developed out of the damaged surfaces. The interpretation of the results will be supported by molecular dynamics simulations of the initial stages of the wear processes. As a primary outcome the project will thus shed light on the atomistic mechanisms responsible for the detachment of flakes, chips, and other structures, and on the early stages of folding, rolling and other morphological changes. Research in materials science, computational physics and nanoscience will be thus covered in a highly synergetic approach.