ERC Consolidator Grant 2019

Advancing *S*olid Interfaces and *L*ubricants by First Pr*i*nciples Material *De*sign

SLIDE

Friction and wear are common phenomena that impact all applications where moving components are in contact, from micro-electromechanical systems to wind turbines, and result in massive economic and environmental costs. By advancing tribological materials impressive energy savings, and consequent reduction of CO_2 emissions, can be obtained. However, in comparison with other technological applications that rely on materials, tribology is remarkably less advanced and the development of lubricants is still based on trial-and-errors methods. 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 interactions between surfaces in contact and simulate reactions in conditions of enhanced reactivity as those imposed by the mechanical stresses applied.

The goal of SLIDE is to port the material design paradigm based on First Principles Material Discovery to the field of Tribology by the development and applications of *i)* a protocol for harnessing tribochemical reactions to reduce interface friction. SLIDE will focus, in particular, in the development of environmental-friendly alternatives to commercial additives used in engine oils; *ii)* a workflow for high throughput screening of solid interfaces. A public database for the intrinsic adhesion and shear strength of a wide number of materials pairs will be created. Such database will constitute a source of realistic parameters for continuum models, paving the way for *serial* multiscale approaches to tribology, from the electronic- to the macro scale. Moreover, with the aid of machine learning algorithms, general trends will be identified and rational ways to chemically modify interfaces for advanced applications will be identified.