Advancing Solid Interfaces and Lubricants by First Principles Material Design

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Friction and wear are common phenomena that impact all the applications where moving components are in contact, and result in massive economic and environmental costs. By advancing tribological systems impressive energy savings, and consequent reduction of CO_2 emissions, can be obtained. However, the performances of lubricant materials are ruled by molecular-level processes that occur at the buried interface, which is 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 materials in conditions of enhanced reactivity as those imposed by the mechanical stresses applied.

I will present the results of ab initio and machine learning molecular dynamics simulations that show how slippery layered materials can be synthesized at the tribological interface thanks to tribochemical reactions. In particular, I will show that selenide layers can be formed by sprinkling Se nanopowders onto sliding contacts [1] and graphene can be obtained by the tribologically-induced polymerization of aromatic molecules [2]. Finally, I will discuss the potentiality of machine-learning interaction potentials to design self-assembled monolayers as friction modifiers [3].
In the second part of the talk I will present TribChem, a software for the high-throughput study of solid interfaces [4], and the results that were obtained for pristine, chemically modified metal-metal, and metal-diamond interfaces [5,6,7].

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These results are part of the "Advancing Solid Interface and Lubricants by First Principles Material Design (SLIDE)" project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant agreement No. 865633).