AB INITIO STUDY OF LUBRICANT MATERIALS

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Understanding and control of friction are key topics in manufacturing and in any application with parts in relative motion, with huge implications, e.g. in the automotive sector, where friction causes the loss of about 70% of the fuel overall energy output. The technologies nowadays available to reduce friction are based on materials, such as solid and liquid lubricants and hard coatings. The functionality of these materials is deeply affected by chemical processes occurring at the sliding buried interface, which are difficult to monitor by experiments. Simulations can play a very important role in their understanding, in particular ab initio molecular dynamics.
We applied this approach to elucidate fundamental mechanisms in the tribochemistry of lubricant additives and diamond like carbon (DLC) coatings used in automotive applications. I will also describe a computational protocol that we developed to calculate from first principles the adhesion and resistance to sliding of solid interfaces. The protocol has been implemented as a software, based on Aiida platform, that allows to obtain the tribological figures of merit in a high throughput way.