Ab initio investigation of atomistic mechanisms in solid and boundary lubrication

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I will present three examples where ab initio calculations have been applied to elucidate atomistic mechanisms in lubrication. The first two studies concern lubrication by chemical surface modifications, while the third example focuses on lubrication by lamellar materials.

Tribochemical reactions can highly influence the tribological properties of materials as they chemically modify the surfaces in contact with consequent modification of their adhesion, resistance to wear and friction. One example is the environmental dependence of the tribological behavior of carbon films: different experiments indicate that the key mechanism for ultralow friction of diamond and hydrogen-free carbon films is the surface passivation. We applied ab initio molecular dynamics as probing tool into the chemical processes occurring at the buried sliding interface of diamond. We identified the mechanisms of surface passivation by water and discuss the effects of the tribological conditions on reaction rates. A second example is the functionality of chemical additives included in engine oils to reduce friction in conditions of boundary lubrication. We identified the reaction paths for S and P release from the dissociative adsorption of model molecules for organo-phosphorous/-suphur additives and analyzed their effects in reducing the adhesion and shear strength of iron interfaces. The results are discussed with reference to corresponding experiments of gas phase lubrication.

Lamellar materials like graphite and molybdenum disulfide are known to be good solid lubricants. In micro- and nano-scale applications, the thickness of a solid lubricant can be a very important factor not only in view of the relative mass of material involved, but also in view of substrate functionalities that can only be preserved by ultrathin layers. We considered few-layer films of graphene and MoS2 and studied the mechanisms of interlayer displacements as a function of thickness. We also evaluated the effects of an applied load by analyzing interlayer electronic charge displacements.