

Towards a universal framework to describe and control atom-scale friction

Macroscopic friction is the result of the interplay of several processes occurring at different scales. At the moment, there is no theory which tells us what is the friction coefficient given the atomic description of two surfaces in contact. The control of friction and the design of new tribological materials with target friction response can then be hardly obtained by using purely experimental models. Also, it is auspicious that friction can be controlled on-the-fly by the user, e.g. by means of electric fields or light irradiation (photofriction). In these latter cases, quantum mechanical effects have to be included in the models. An atomic scale definition of friction is therefore mandatory to provide a deep and, possibly, complete understanding and control of the underlying phenomena.

The aim of the present work is to extract information on the frictional and dissipative response of a system from the only knowledge of its static properties at the atomic level, without the need to perform long and costly dynamic simulations. In parallel, the challenge is to develop a quantum mechanical system-independent framework which is applicable to any kind of chemistry and atomic topology. To achieve this, the friction response is recast in terms of suitable phonon modes and related scattering tensor elements. This approach allows to control the frictional properties of existing materials in a subtle way; at the same time, the approach suggests how to design new tribological materials with target frictional response.

The result of this method is a phonon-based friction theory, where the phonon theory and the quantum mechanics have been used to pave the way towards a universal framework to describe and control friction occurring at the atomic scale. It is then expected that this work may pave the way towards a phonon friction theory which can tackle one of the biggest challenges of nanotribology: the calculation of the friction coefficient of two interacting surfaces based on the sole knowledge of the atom types and their geometric arrangement.