Simulation of Processes @ quasi-2D Interfaces by ab initio MD

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Abstract

The modeling of nanostructures by means of atomistic simulations, often based on density functional theory, has become a key ingredient to gain insight on the properties of fascinating and complex new materials. Such theoretical studies are often able to highlight aspects that successively can be exploited to design new systems and to advance their application. Since long, our research activity has been dedicated to the development and improvement of suitable computational protocols to address the always new challenging questions that keep arising from the experimental side. The implementation of efficient and strongly parallelized algorithms has allowed to extend the scope of molecular simulation, also straddling over several levels of theory and length scales. The diversification of methods and models is essential to tackle problems of increasing complexity. We specialized, in particular, on quasi two dimensional materials formed at the surface of crystalline solids, and on their interaction with atoms, clusters, or molecules. Thanks to the input received from the close collaboration with different experimental groups and also investing in the constant further development of our high performance condensed matter simulation package, our research is state of the art in addressing large scale electronic structure problems combined with structural refinements and molecular dynamics. Advanced material science studies of the type that we propose would neither be possible without the exchange with the experimental partners nor without adequate computational resources.