Atomistic quantum simulation of materials using the Density Functional based Tight-Binding Method

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Atomistic simulations are becoming an essential tool in the study of the physical and chemical properties of materials. Depending on how the interatomic interactions are considered, the atomistic techniques can be based on classical (empirical methods) or quantum approximations (ab initio and semi-empirical methods). The former allows the investigation of materials in realistic thermodynamical conditions, on millions of atoms. However, empirical methods can fail when some surface and quantum effects are dominant phenomena. In contrast, *ab initio*, or first-principle methods, have been implemented successfully to describe the full quantum electronic structure of many materials, but only for a few hundred of atoms.

Semiempirical methods offer an interesting alternative, being more than three order of magnitudes faster than methods based on the Density Functional Theory (DFT), which are the fastest *ab initio* method available. The so-called Self-Consistent Charge Density-Functional Tight-Binding (SCC-DFTB) method has been widely applied to model the structure, excited states and electronic transport, among many other physical and chemical properties, for various materials. In this talk I will introduce the SCC-DFTB method and show some results that we have obtained with this technique for the structural and vibrational properties of silica glasses, and for metal nanoparticles and their plasmonic resonances. Additionally, some preliminary results on OH- Graphene functionalization and the molecular diffusion of glucose-water mixtures will be presented.