PhD Thesis Summary

Computational study of reduced Graphene Oxide properties for membrane applications

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In this doctoral thesis we used state-of-the-art atomistic simulations to model and investigate the electronic properties of reduced Graphene Oxide, its structural evolution upon annealing and the properties of the interface that it forms with water. Reduced GO (rGO) is a very versatile material, atomically-thin as graphene but with much higher complexity due to its variable composition. It is fabricated oxidizing graphite, a treatment that induce complex modifications to the structural and electronic properties of this material that are still not completely understood.
In this work we try to address some important questions that are still open in GO literature, in particular we presented the results of a thorough computational investigation of the structural and electronic properties of rGO, based on accurate classical MD and DFT simulations. Based on these simulations, we suggested a modification to a widely used structural model for GO and provided useful indications to help with interpretation XPS C1s spectra. Moreover, we discussed the mechanisms that lead to oxygen-containing species to diffuse and clusterize in monolayer rGO and investigated how to control this phenomenon to exploit it for producing pores of controlled size. In fact, we provided reliable indications to produce porous single layer rGO membranes for water filtration in a scalable and controllable way. Finally, we investigated the interactions between water and rGO and studied how its composition influences surface wettability. We concluded this research project studying the effects of confinement on water between rGO flakes, considering a realistic interlayer distance between the latter as observed in multilayer rGO membranes when soaked in water. Conclusions from this work will shine light on the relationships between microscopical features of rGO flakes and the diffusivity of water molecules in their proximities, fundamental to engineer efficient membranes for water desalination.