Exploring the real nano-world using HPC beyond the ab-initio approach

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The advances in the predictive power, speed and reliability of ab-initio methods has occurred in the last few decades at a very fast pace. Simultaneously, the computing power available through HPC facilities has continued growing exponentially. This combination has brought the paradigm of ab-initio simulations as an invaluable tool to understand and predict the behavior of matter at the nanoscale. However, enormous challenges are still ahead of us, to be able to extend the range of practical applicability of these methods to the sizes and time scales which are relevant to most of the practical problems in nanotechnology. In this talk, I will talk about some of these challenges, and discuss strategies to use the information extracted from ab-initio simulations to tackle problems in the length and time scales which are really relevant for practical uses of nanotechnology. In particular, I will describe approaches to study electronic transport properties in nano-to-meso scale devices (see Figure 1) [1], and the interaction of large proteins with inorganic nanostructures. The role of HPC facilities and the interaction between these and the development of simulation tools will also be discussed [2].

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References

[1] N. Leconte, J. Moser, P. Ordejón, H. Tao, A. Lherbier, A. Bachtold, F. Alsina, C. Sotomayor Torres, J.-C. Charlier and S. Roche, ACS Nano **4** (2010) 4033
[2] C. F. Sanz-Navarro, R. Grima, A. García, Edgar A. Bea, A. Soba, J. M. Cela and P. Ordejón, Theor. Chem. Acc **128** (2011) 825

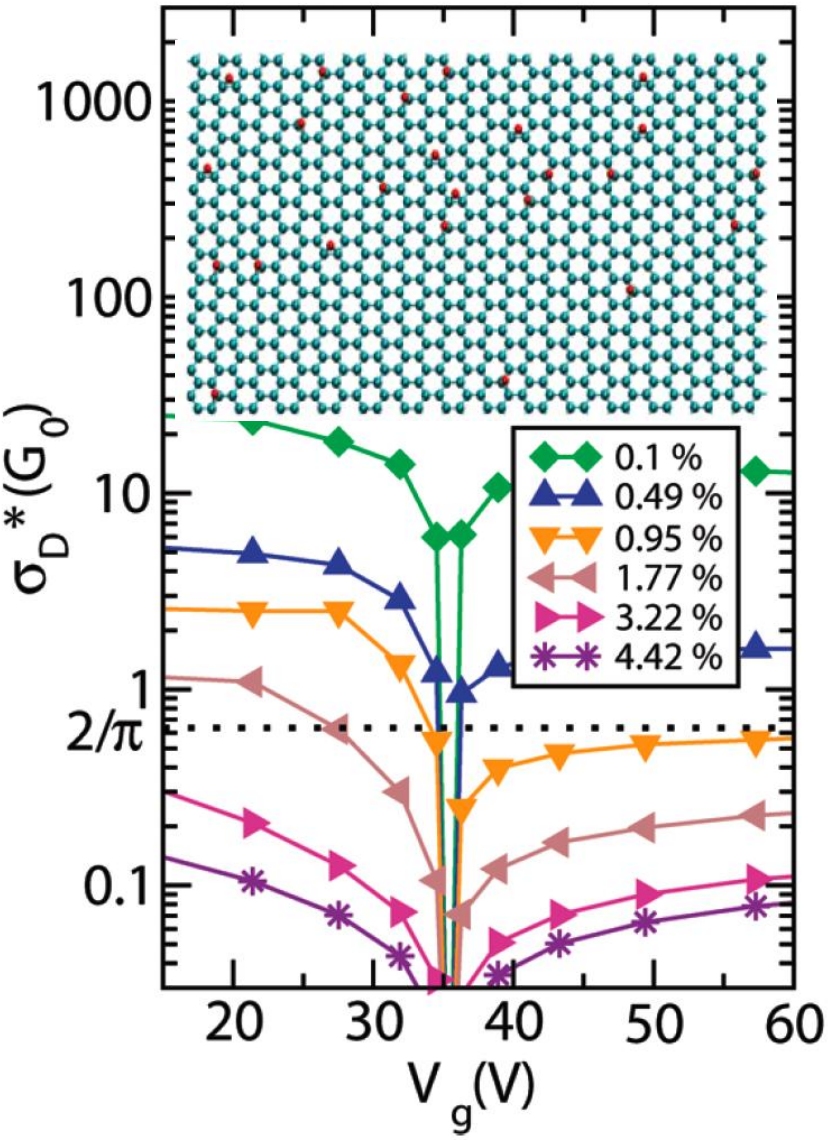

Figure 1. Drude conductivity of samples of graphene functionalized with different concentrations of oxygen, in the configuration of epoxide groups, as a function of gate voltage. The inset shows a section of one of the samples. Adapted from Ref. [1]