Exploring nanoscale materials with Density Functional Theory: probing structural mechanical and electronic properties

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In the last decades, Density-Functional-Theory (DFT) has been established as the cornerstone method for the study of the electronic structure of materials, and for the exploration of materials properties at the nanoscale. This presentation provides a review of DFT approximations as well as their most popular computational implementations. We will discuss the strengths, but also the limitations and challenges of these approaches. One such striking challenge is the accurate prediction of electronic properties like the band gaps of semiconductors. To illustrate the versatility of DFT, we will present applications to several systems of present day scientific and technological interest.

Such applications include: (a) Investigating the structural and dynamic stability of recently proposed cage molecular structures; (b) Predicting the performance of single-layer, graphene-based, nano-porous membranes for gas separation, by performing transition state calculations and combining with the kinetic theory of gases; (c) Probing the electronic properties of systems of particular interest for photovoltaic and optoelectronic applications. Such systems include metal oxides (like Cu_2O) and perovskites of the form A_2ZrX_6 (where A is one of $(CH_3)_3S^+$, $CH(NH)_2^+$, or $CH_3NH_3^+$, and X = Cl, Br, or I). In that study we employed semi-local and hybrid DFT approximations. Our goal was to investigate the effect of different compositions and doping on the optoelectronic properties. By focusing on these diverse applications, we aim to demonstrate the power of DFT in addressing important problems and challenges in materials science.