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Curriculum Vitae

Publications and Reprints

Research Interests

My work refers mainly to ab-intio molecular dynamics. In particular, during my PhD I studied the interaction between grafene and Cr atoms or dimers. This work was motivated by some recent experimental results that showed that the elastic shear modulus of multi wall carbon nanotubes (MWCNT) under repeated twisting cycles saturates to a value about ten times larger than the initial one. Since a Cr gas is evaporated on MWCNTs in the fabrication of experimental devices, it seemed resonable that Cr played an important role. Moreover the formation and activation energies of Stone-Wales or vacancy defects in graphene are too large to be considered alone in this situation. We found various stable configurations of Cr atoms and dimer on graphene, both defective or not, and studied a possible mechanism by which a Cr dimer can be intercalated trough graphene sheets and than dissociates.

Current Research Projects

- **Sodium alanates as hydrogen storage material** Sodium alanates ($NaAlH_4$) are among the best candidates for solid state hydrogen storage. Recent experimental results, obtained using anelastic spectroscopy and other methods, suggested the presence of an highly mobile entity created during the first de-hydrogenization reaction in sodium alanate. The experimentalists proposed the following explanation of the observed highly mobile entity: during the reaction, defective units of AlH_6 group are formed and the signal is due to a local (that is around the defective AlH_6 group itself) migration of the vacancy. We are working to define a (set of) good collective variable to describe this process so as to study by ab-initio molecular methods the activation energy of the motion and compare it with experimental results.

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