Ab initio calculations of electronic and transport properties of disordered one-dimensional carbon systems

da Silva, A. J. R.[(1)*]

Instituto de Física – Universidade de São Paulo, São Paulo, SP, Brazil ajrsilva@if.usp.br

Nanoscale carbon-based materials have been on the spotlight for two decades, starting with fullerenes, then carbon nanotubes (CNTs) and more recently graphene sheets and nanoribbons (GNRs). The understanding of the electronic transport properties of CNTs and GNRs devices presents tantalizing possibilities. Both materials have exceptional transport properties which can be affected by the presence of defects and impurities [1-3]. For example, it has been demonstrated that carbon nanotubes can be used as sensors for hazardous gases. Large scale computer simulations have an important role to play in predicting the transport properties of such systems. In order to do so it is important to have the ability to: 1) understand the detailed properties of individual defects, with the identification of the most relevant ones; 2) study the charge transport properties of the individual, isolated, defects; 3) and finally and most importantly, to provide a full description of a large scale system, with disorder taken into account. In this talk I will illustrate how calculations based on Density Functional Theory and recursive Greens functions techniques can in some cases provide such a framework [4]. Two particular examples will be discussed: 1) nitrogen-doped CNTs, which can act as ammonia sensors; and 2) boron doped GNRs, which may lead to spin filter devices.

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