Graphene nanoflakes: Energy gap engineering and vacancy-induced magnetism

The electronic structure of graphene corresponds to a semi-metal with p-electrons at Fermi level, which are responsible of the unique electronic properties for this material. Graphene nanostructures show an energy gap resulting of the finite size, and are of current interest because of the potential applications in electronic and optoelectronic devices. Thus, we discuss some recent progress in the synthesis of graphene nanoflakes obtained from the reaction of polyaromatic hydrocarbons and from fullerenes or nanotubes. In this talk, we are presenting ab-initio results for the electronic properties of graphene nanoflakes of different effective radius (R) and different shapes. We find that the Kohn-Sham gap decreases with size as R⁻¹, as predicted by the simple confinement model, while the quasi-particle energy gap follow the R⁻⁰.₈ scaling rule. Secondly, the electronic structure of graphene nanoflakes with edge chemical modifications using different atoms and functional groups is analyzed. The results suggest the feasibility of tailoring the electronic and optical properties of graphene nanostructures by edge doping. Finally, the problem of determining the magnetic moment of graphene nanoflakes with single-vacancy defects is addressed. Using the Fixed Spin Moment method, the ground state spin multiplicity and the spin magnetic distribution was obtained. We found that the ground state multiplicity is triplet, corresponding to a spin magnetic moment of 2 μB. From the analysis of the orbital spin distribution we found that the spin-polarized is equally distributed in the sp² and pz orbitals. The nature of the sp-magnetism in these carbon nanostructures is discussed. Work supported by Conacyt-México under Grant No. 83604.