Alejandro López-Bezanilla

Postdoctoral Research Associate
Center For Nanophase Materials Sciences Division
Oak Ridge National Laboratory
(865) 574-7192
alm@ornl.gov

Education

Universidad Autónoma de Madrid, Spain	Physical Sciences	Licenciado, 2006
Ecole Doctoral de Grenoble, France	Computational Physics	Ph.D., 2009

Professional Experience

2010- present	Postdoctoral Research Associate, American Recovery and Reinvestment Act Fellow, Center For Nanophase Materials Sciences, Oak Ridge National Labratory.
2006-2009	PhD student , Marie Curie European Fellowship, Groupe Thèorie at INAC, CEA-Grenoble.
2004	Internship, L_Sim Laboratory at INAC, Commissariat à l´Energie Atomique -Grenoble.

Publications (Over 10 publications including 1 review, 1 encyclopedia chapter, 1book chapter)

Research Synopsis

1. *Quantum Transport Properties of Modified Graphene Nanoribbons*.
   We use electronic structure calculations based on the density functional theory to explore the electronic quantum transport properties of graphene nanoribbons modified with functional groups such as O atoms, BN domains and sp^3 surface defects. The Green function formalism and the decimation technique for the real space normalization allow for the study of realistic long systems from the accuracy of first-principles calculations.
2. *Electronic Structure Calculations of BN Nanoribbons*.
   Density functional theory simulations are used to explore the electronic and geometrical properties of boron nitride nanoribbons with different edge terminations.
3. *Electronic Transport Properties of Functionalized Carbon Nanotubes.*

   By means of electronic structure calculations based on *ab initio* tools coupled with the Landauer-Büttiker approach for one-dimensional electronic transport, we predict the transport properties of functionalized carbon nanotubes at the mesoscopic scale.
4. *STM simulations of polymers in π-staking*.
   We use solid state electronic structure calculations and the Tersoff-Hoffman parametrization approach to characterize the π-π stacking mechanism of π conjugated polymers.