

University of Pittsburgh

Petersen Institute of NanoScience and Engineering Seminar

Speaker: Professor Angel Rubio

Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility, Universidad del País Vasco, San Sebastián, Spain

Title: *Boron Nitride and Graphene Nanostructures: Properties and Applications*

Time/Date: 12:00 noon, Tuesday, March 17, 2009
(refreshments at 12:00noon - 12:15pm)

Place: Kresge Conference Center, 1175 Benedum Hall

We will review the work done in the group in the last year to characterize and predict the properties of boron-nitride-based nanostructures and address their potential applications, in particular the different spectroscopic techniques that are currently used for boron-nitride nanostructures. We will present the spectroscopy of hexagonal boron nitride (hBN) (sheet and bulk) and BN nanotubes from a theoretical perspective. The measured Raman spectra can be fully explained by ab-initio simulations of the spectra. For the interpretation of optical absorption and luminescence, a detailed knowledge of the excited state properties is required. We show that BN displays strongly bound excitons whose binding energy increases from three-dimensional hBN, via the 2D single sheet to the quasi-1D BN tubes. However, the excited state properties of the pure structures seem not to explain most of the measured luminescence spectra. Thus, we investigate the influence of different possible defects in hBN such as vacancies and carbon substitutions. Furthermore, we present results on the influence of external E-fields on the excitonic spectra of BN tubes. We will discuss potential applications of BN in optoelectronic devices as well as other application in combination with C-tubes. We will summarize the experimental and theoretical studies in those structures and at the end we will make connections with carbon-based materials, as graphene/graphite and their interconnections.

Biographical Sketch

Dr. Angel Rubio is a Professor of Condensed Matter Physics at the Departamento de Física de Materiales, Facultad de Químicas, Universidad del País Vasco, and member of the Unidad de Física de Materiales Centro Mixto CSIC-UPV/EHU. He is Distinguished Visiting Scientist and Group Leader for Theoretical Spectroscopy at the Fritz Haber Institute der Max-Planck-Gesellschaft, Berlin. Dr. Rubio also serves as the Vice-President for Scientific Development, European Theoretical Spectroscopy Facility. Prof. Rubio's major research interests are in condensed matter physics and nanoscience, in particular, the description and prediction of the electronic structure, spectroscopic and transport properties of nanoscale materials and biological

systems. Those studies include studies related to the fundamentals of many-body perturbation theory and static as well as time-dependent density functional theory (DFT and TDDFT); with application to a large class of systems from nanotubes, nanostructures, biological molecules (photoreceptors), transport in molecular devices. For further information on these topics visit the page on <http://nano-bio.ehu.es>.