Título: Curved Carbon Nanostructures: From graphene to Fullerenes and Schwarzites
Prof. Dr. Humberto Terrones (Department of Physics, Rensselaer Polytechnic Institute, NY, USA)
Data: Quinta-feira 30/07/2015
Horário: 15:00 h
Local: Auditório do Departamento de Física

Resumo: Since the first X-Ray diffraction pattern studies of Peter Debye, Paul Scherrer and Albert W. Hull in 1917 it was known that graphite was composed of hexagonal layers of sp2 carbon, known today as graphene layers. The main point at this time was to address the issue of how the graphene layers were stacked to
form the 3-D crystal of graphite. In 1924 John Desmond Bernal found that the stacking of hexagonal layers in graphite could be of the type A-B-A-B, known now as Bernal graphite. It was in 1985, with the discovery of C60 or Buckminsterfullerene by Harold Kroto, Robert Curl, Richard Smalley, Jim Heat and Sean O'Brien, that two main important points were brought into scene: First, that molecules could be formed out of one layer of graphite (graphene), and second, that this layer could acquire curvature. Bearing this in mind, in 1991 Alan L. Mackay and Humberto Terrones by using differential geometry concepts put into context the different shapes that graphenic structures could possess adding to the Fullerenes a new family of graphene foams named Schwarzites which structure could be achieved by the introduction of sp2 carbon rings with more than six carbon atoms. Nowadays with the possibility of synthesizing in a controlled way an isolated graphene sheet, researchers have re-started to implement methods which could generate other shapes including Schwarzites which have remained elusive. In 2015, Yingpeng Wu and colleagues were able to obtain a spongy graphene with very interesting mechanical properties such as almost zero Poisson ratio. In this talk, besides reviewing the basic studies
related to different possible shapes of graphene involving Fullerenes, carbon nanotubes and Schwarzites, recent calculations on giant Schwarzites will be presented to shed light on their new electronic and mechanical properties. It has been found that Dirac hyper-cones can be present in giant Schwarzites and that the Poisson Ratio can be reduced, not only to zero, but also to negative values,
thus opening new possibilities for curved nanostructures.

Título: Beyond Graphene: The amazing world of layered transition metal dichalcogenides
Prof. Dr. Humberto Terrones (Department of Physics, Rensselaer Polytechnic Institute, NY, USA)
Data: Sexta-feira 31/07/2015
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Local: Auditório do Departamento de Física

Resumo: Graphene, an atom thick of carbon semimetal, has attracted a great deal of attention due to its new properties and promising applications which might have impact in new electronic devices, novel composite materials, innovative sensors, etc. However, graphene it is not alone, there is also hexagonal boron nitride (H-BN) a layered insulator which can be combined with graphene to form new hetero layer materials. Moreover, there are flat layered structures made out of transition metal dichacogenides (TMD) such as MoS2, WS2, MoSe2, WSe2, NbS2, NbSe2, WTe2, etc., which can behave as semiconductors or metals depending on the atoms involved. Interestingly, one monolayer of a semiconducting TMD exhibits a direct band gap which vanishes when adding another layer, thus producing an indirect band gap bilayer material. Since monolayer semiconducting TMD, with trigonal prismatic structure, do not possess center of inversion, exhibit valley polarization effects which envisage their application in non-linear optics and in a new field called valley-tronics. In this talk, theoretical and experimental efforts to shed light on the comportment of TMDs will be provided. First, the main synthesis methods of monolayer TMDs such as exfoliation, chemical vapor transport and chemical vapor deposition will be studied along with their main challenges. Second, the role of defects and doping of TMDs will be analyzed, and finally, first principles calculations to understand their opto-electronic behavior and Raman scattering will be also explained.