



School of Nano Science



IPM Condensed Matter &
Statistical Physics Group

Weekly Seminar

Raman and IR spectroscopy for applications in nanographenes

Invited speaker: **Dr. Ali Maghsoumi**

Postdoctoral Scientist, Sharif University of Technology

Abstract:

This speech focused on the use of vibrational spectroscopy for the characterization of advanced molecular materials appealing for applications in molecular electronics due to the electronic and optical properties imparted by the presence of conjugated π -electrons.

Graphene molecules constitute effective models of graphene confined over a limited region. They are well defined cutouts or model compounds of graphene and graphene nanoribbons. Due to confinement, the electronic and vibrational properties of graphene molecules can be modulated, leading to functional molecules optimized for specific applications.

π electrons of conjugated materials are the key actor in Resonance Raman (RR) spectroscopy, which is an effective probe of both the electronic and the vibrational properties. Hence the experimental pre-resonance/resonance Raman response of a representative graphene molecule (C78) has been investigated based on the recently developed approach to the calculation of RR response of π -conjugated molecules. The outcomes of this analysis can be extrapolated to graphene, for which Raman spectroscopy is one of the more commonly used characterization techniques.

Among graphene molecules, Hexa-peri-hexabenzocoronene (HBC) is one the most important examples of the fully benzenoid PAHs. Raman and IR spectroscopies have been used to characterize and prove the chemical structure of tetrazigzag-HBC, selected graphene nanoribbons (GNRs) and their monomers, chlorinated molecular graphenes and a model molecule of a "hole" in graphene.

Furthermore, IR spectroscopy was used to investigate and find different edge markers or functionalisation markers. From this point of view, IR spectroscopy is complementary to Raman spectroscopy for which the signals are mostly due to the collective motions involving the molecular π -conjugated core and usually carry less information on functional groups.

Wednesday, 10 Mordad 1397 (Aug 1, 2018), 14:00-15:00

Seminar Room (classroom A), Farmanieh Building, IPM