



School of Nano Science



IPM Condensed Matter &  
Statistical Physics Group

## Weekly Seminar

# Localized charge fragments for efficient, “on-the-fly” calculation of vibrational spectra and many-body dispersion interactions in density-functional theory

Invited Speaker:

**Dr. Pouya Partovi-Azar**

Freie Universitaet Berlin, Germany

### Abstract:

In the first part of the talk, I will present a novel computational method to accurately calculate Raman spectra from first principles. Propagating maximally localized Wannier functions (WF) in time together with the nuclei, this method is about an order of magnitude faster than those employing finite-differences method to calculate the polarizability. This scheme thus allows to routinely calculate finite-temperature Raman spectra “on-the-fly” by means of ab-initio molecular dynamics simulations. I will then present the results on the effect of hydrophobic and hydrophilic solutes in water solution on the infrared and Raman spectra. Afterwards, I will demonstrate the predictive power of the new method, specially the ability to decompose the total vibrational spectra into local contributions, to elucidate the reversible transition mechanism of lithium polysulfide formation in lithium-sulfur batteries.

In the second part, I will focus on long-range dispersion interactions, a many-body correlation effect which is usually neglected in conventional DFT calculations based on local approximations to the exchange and correlation effects. I will introduce the semi-empirical as well as first-principles approaches proposed so far to correct the DFT calculations. Then I will introduce the many-body dispersion (MBD) approach, and will demonstrate how a WF-based picture can be utilized to calculate the correction. I will end the talk by presenting our results on water adsorption on graphene single- and bilayers, obtained by an extension to the original WF-based MBD for periodic systems. It will be shown that the dispersion interactions can be, in some cases, repulsive.

Wednesday, 10 Shahrivar 95 (31 August, 2016), 2-3 pm

Farmaniyeh seminar room