Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Wednesday, January 18th 2017 - 11:30
CFEL Seminar room IV (Bldg. 99)

Enrico Ronca

California Institute of Technology, Pasadena, CA, USA

Theoretical Methods for Excited State Properties in Extended Systems

Light matter interaction is involved in several fundamental processes in Chemistry, Physics and Biology and is at the basis of Spectroscopy, experimental technique representing probably the most important source of information about properties of matter. Due to the significant improvements introduced in the last decades, spectroscopic techniques became very accurate and the interpretation of spectra, just by observation of the experimental results, became sometimes extremely complicated. For this reason the need of accurate theoretical methods able to reproduce and interpret the experimental results is becoming more and more pressing. The accurate theoretical simulation of spectra is therefore a very a challenging task, in particular for extended systems for which only approximated methods can be used.

In this talk I'll presents some of the theoretical methods I developed during my research activity to improve the description of excited state properties (spectra, densities, charge transfer ...) in extended chemical and physical systems.

The first part of the talk will be mainly focused on methods able to improve the description of charge transfer states at a reasonable computational cost. Applications in the field of hybrid photovoltaic and light harvesting in general will be presented.

The second part of the talk will be focused instead on recent methods, based on the Density Matrix Renormalization Group (DMRG) numerical technique, I developed to simulate spectra of strongly correlated systems.

Host: Angel Rubio

MAX-PLANCK-GESELLSCHAFT