Department of Physical and Theoretical Chemistry & Department of Inorganic Chemistry
are cordially inviting you to a joint seminar

22 February 2016, 13:10

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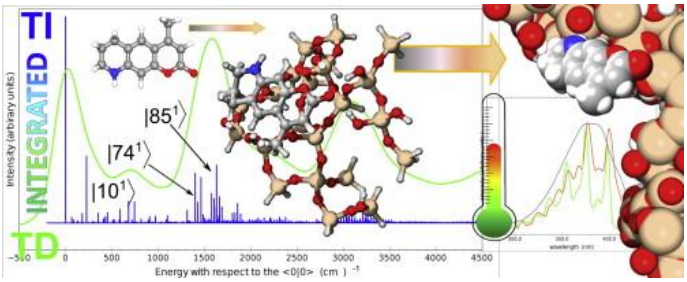

Dr. Luciano Carta
University of Napoli – Federico II, Italy

Modern DFT and TD-DFT approaches applied to real life

We will look at efficiency of DFT and TD-DFT calculations as applied to many cases, e.g. from cultural heritages to smart materials, Li-Ion batteries and solar cells. We will focus on simulation of electronic structure, which can be directly compared with experimental results. In this respect, it has been possible to describe electronic and structural characteristics of free molecules in different environmental conditions, for which experimental spectroscopic data are available, and then extend such studies towards similar targets, taking into account all the different effects.

From a general point of view this type of studies underlines the ability of modern computational approaches to provide an in-depth comprehension of the nature, behavior and the composition of various materials and at the same time allow us to understand the physics/chemistry of such microscopic processes.

Prof. I. Černušák

Head of the Department of Physical
And Theoretical Chemistry

Prof. J. Noga

Head of the Department of
Inorganic Chemistry