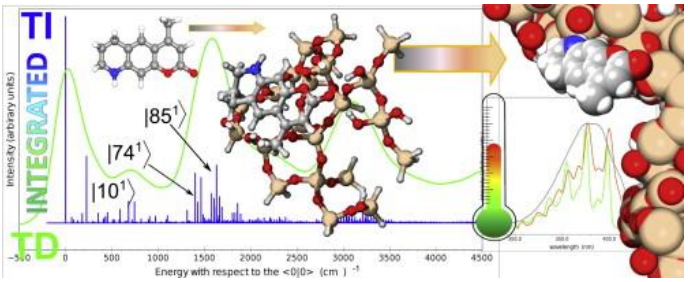
Katedra fyzikálnej a teoretickej chémie a Katedra anorganickej chémie
Vás srdečne pozývajú na spoločný odborný seminár

22. februára 2016, 13:10

V knižnici Katedry anorganickej chémie (CH2-213)



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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

Vedúci Katedry fyzikálnej
a teoretickej chémie

Prof. J. Noga

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