Contribution (Keynote)

(Imaginenano 2011 Extended abstract format: 2 pages max including figures and references. Font: Arial 10, use line spacing single. Please follow the model below.)

Modeling Photo-induced dynamical processes in massive parallel architectures

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There has been much progress in the synthesis and characterization of nanostructures however; there remain immense challenges in understanding their properties and interactions with external probes in order to realize their tremendous potential for applications (molecular electronics, nanoscale opto-electronic devices, light harvesting and emitting nanostructures). In this talk we will review the recent advances within density-functional based schemes to describe spectroscopic properties of those complex systems. Special emphasis will be made in modeling new materials and simulate new time and spatially resolved spectroscopies. We will address both linear and non-linear response regimes to study the optical absorption and luminescence of bio-chromophores, one-dimensional polymers and nanotubes and layered materials. Moreover, we will illustrate how an optimal control theory can be implemented such that we could have control of the quantum state of a molecular structure.

Within the goal of spanning larger time-scales and more complex structures, we will describe a new method to mimic the electron-ion dynamics within the Ehrenfest scheme where no explicit orthogonalization is necessary and we can increase of the time step while keeping the system close to the Born-Oppenheimer surface. The method is easily implemented and scales very well with the system size. Applications to the excited state dynamics in some organic molecules will be used as text cases to illustrate the performance of the approach. We will present the dynamical processes in organic/inorganic charge-transfer systems and biological complexes. In particular we will show the effect of electron-hole attraction in those systems. Pros and cons of present functionals will be highlighted and provide insight in how to overcome those limitations by merging concepts from many-body perturbation theory and time-dependent density functional theory.

All those developments constitute a basic ingredient for the realization of the European Theoretical Spectroscopy Facility (ETSF, http://etsf.eu) as a top-level scientific infrastructure. We implemented all those ideas in the open source computer code OCTOPUS (http://www.tddft.org) This program released in 2002 simulates the dynamics of electrons and nuclei under the influence of arbitrary time-dependent fields. his code is very versatile and can handle diverse physical situations (molecules, solids, 2D quantum dots, etc.) making it an extremely powerful tool for spectroscopy. Thanks to its current parallel capabilities, OCTOPUS was chosen as a benchmark code for the Partnership for Advanced Computing in Europe[1] (PRACE) initiative that aims to provide European scientists with world-class leadership supercomputing infrastructures

1http://www.prace-project.eu/