CFEL SCIENCE

Colloquium

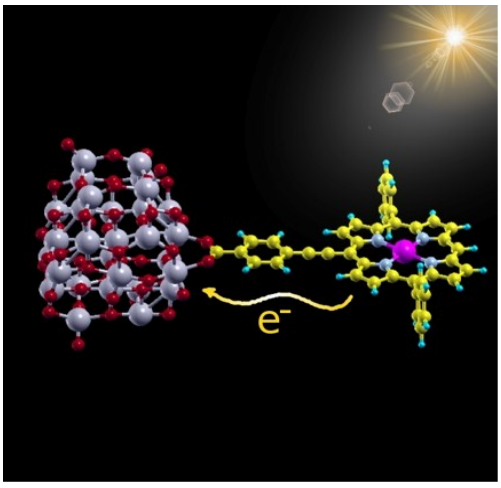
06th July 2012 – 13:15

FLASH HALL, Seminar Room (28c)

Angel Rubio

Universidad del Pais Vasco and Fritz Haber Institute

Modelling photo-induced dynamical processes in nanostructures and biomolecules from first principles: correlation effects and applications



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 electron spectroscopies (including transient pump-probe techniques). We will address, within the time-dependent density-functional theory (TDDFT) framework [1,2] both linear and non-linear response regimes to study the optical absorption, luminescence and photoelectron spectra of bio-chromophores, one-dimensional systems and layered materials as well as the dynamical processes in organic/inorganic charge-transfer systems. As an illustration of the techniques we will focus on two relevant examples, one linked to the efficient conversion of light into electricity or chemical fuels ("artificial photosynthesis") [3] and the other to the design of new nanostructured based optoelectronic devices based on inorganic nanotubes.

[1] M.A.L. Marques, N. Maitra, F. Nogueira, E.K.U Gross, and A. Rubio (Editors) “Fundamentals of Time-Dependent Density Functional Theory" Lecture Notes in Physics, Springer Verlag Vol. 837 (2012)

[2] A. Castro, H. Appel, M. Oliveira, C. A. Rozzi, X. Andrade, F. Lorenzen, M. A. L. Marques, E. K. U. Gross and A. Rubio, octopus: a tool for the application of time-dependent density functional theory, Physica Status Solidi (b) **243** 2465-2488 (2006); X. Andrade, J. Alberdi-Rodriguez,, D. A Strubbe, M.J T Oliveira,F. Nogueira, A. Castro, J. Muguerza, A. Arruabarrena, S.G Louie, A. Aspuru-Guzik, A. Rubio, and M.A.L. Marques, Time-dependent density-functional theory in massively parallel computer architectures: the octopus project, Journal of Physics: Condensed Matter **24** 233202-1,11(2012)

[3] Quantum coherence controls the charge separation in a prototypical artificial light harvesting system Carlo Andrea Rozzi, Sarah Maria Falke, Nicola Spallanzani, Angel Rubio, Elisa Molinari, Daniele Brida, Margherita Maiuri, Giulio Cerullo, Heiko Schramm, Jens Christoffers & Christoph Lienau (submitted for publication)

Host: Robin Santra - CFEL Theory Division