TDDFT for nonlinear phenomena of light-matter interactions
ANGEL RUBIO, NanoBio Spectroscopy Group and ETSF Scientific Development Centre, Faculty of Chemistry University of the Basque Count

Despite the success of linear-response schemes to describe excitations of many electron systems, many physical processes stemming from the interaction of light with matter are nonlinear in nature. In this talk we will address the problems and open questions related to the description of this phenomena with the goal of providing a sound description of laser-induced-population processes within TDDFT. Through the exact solution of a few electron system interacting with a monochromatic laser we highlight some common deficiencies of all adiabatic density functionals within time-dependent density-functional theory to handle photoinduced processes leading to population changes of many-body states. One prototype case is Rabi oscillations between the ground and an excited state when a monochromatic laser with a frequency close to the resonance is applied. All adiabatic functionals are not able to discern between resonant and nonresonant (detuned) Rabi oscillations. Only the inclusion of an appropriate memory dependence can correct the fictitious time-dependence of the resonant frequency. We extend this description to dynamical induced charge transfer processes and many body tunneling. Adiabatic functionals will fail similarly in the description of all processes involving a change in the population of states. We will show our recent advances in deriving a new memory-dependent functional. The description of photo-induced processes in chemistry, physics, and biology and the newfield of attosecond electron dynamics and high-intense lasers all demand fundamental functional developments going beyond the adiabatic approximation.