Ab-initio Real-Time Simulation of Light-Matter Interaction Using TDDFT

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Time-dependent density-functional theory (TDDFT) is the ab-initio method that has been widely used to theoretically study optical properties of large quantum-mechanical systems beyond the computational reach of full quantum-chemical methods (e.g., configurations interaction based ones). As I will discuss in this talk its success relies on its use in time-evolution (or, real-time) formalism. As examples, optical properties of bare and ligand-protected metal clusters, as well as opto-magnetic response in them will be presented. Furthermore, in the context of ultra-fast sub-femtosecond electron dynamics and also in view my proposed research activities in the ILM, I'll talk about the limitations of the present-day use TDDFT and the state-of-art in overcoming them.