# REAL TIME ELECTRON DYNAMICS USING TDDFT

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The correct description of electronic excited states is essential for understanding many physical-chemical properties of great interest, such as charge transport phenomena, spectroscopy, quantum transport and photochemistry. We will present here a first-principle metodology implemented in the code developed by our group that allows us to evolve in real time the electronic density beyond its ground state. Moreover, we are finishing incorporating the possibility of modelling the conjoint but independent movement of the nuclei using an Ehrenfest scheme. These methods use the formalism of DFT and our code can be coupled with the molecular dynamics programs AMBER and GROMACS, which allows us to then perform QM-MM calculations. We will show some applications of these features, including the simulation of the photodissociation of simple molecules that have been electronically excited.

**References**

1) Morzan U. N., *J Chem Phys*, **2014**, 140, 164105.
2) Morzan U. N., *J Chem Phys*, **2016**, 146, 044110.