MODELING LASER-INDUCED MOLECULE EXCITATIONS USING REAL-TIME, TIME-DEPENDENT DENSITY FUNCTIONAL THEORY

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The fully propagated real time-dependent density functional theory (RT-TDDFT) method has been applied to study the laser–molecule interaction in different molecular systems. After a short overview of the RT-TDDFT theoretical model, several real-case applications, including the computing of the full electronic absorption spectrum, resonant and charge-transfer-type excitations, as well as the dynamics of different orbital populations in real time scale will be presented.

The roles of the different laser field parameters, like field direction, strength, and wavelength, or pulse shape are discussed in order to get efficient and selective excitation behaviors for the chosen specific molecular systems [1,2].

At the end some remarks about the advantage and disadvantage of RT-TDDFT as well as about the possible further developments are given.

[1] A. Bende, V. Toşa, Physical Chemistry Chemical Physics, 17 (2015) 5861 – 5871.
[2] A. Bende, Annual Reports in Computational Chemistry, Vol. 11, (2015) 103 – 146.