Attosecond pump-probe spectroscopy of molecular electron dynamics: a theoretical point of view

Fernando Martín^{1,2,3.}

¹Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, 28049 Madrid, Spain.

²Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nano), Campus de Cantoblanco, 28049 Madrid, Spain.

³ Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain.

fernando.martin@uam.es

Attosecond and few femtosecond light pulses allow one to probe the inner workings of atoms, molecules and solids on the timescale of the electronic motion. In molecules, sudden ionization by such pulses is followed by charge redistribution on a time scale ranging from a few-femtoseconds down to hundreds attoseconds, and usually leads to fragmentation of the remaining molecular cation. Such complex dynamics arises from the coherent superposition of electronic states populated by the broadband attosecond pulse and from rearrangements in the electronic structure of the molecular cation due to electron correlation. To investigate these ultrafast processes, attosecond pump-probe spectroscopy has been shown to be a very valuable tool. In this talk I will present the results of recent attosecond pump-probe simulations in which several atoms and molecules, from hydrogen to the amino acid tryptophan, are ionized with a single or a train of attosecond pulses and are subsequently probed by an infrared or an XUV pulse (see [1] for a recent review on the subject).

[1] M. Nisoli, P. Decleva, F. Calegari, A. Palacios, and F. Martín, Chem. Rev. **117**, 10760 (2017).