Evolution of the Electronic Coherences Induced by an Initial Pulse Through Nuclear Quantum Dynamics

M Alías-Rodríguez[1], C González-Collado[2], A Palacios[2], and F Martin[1,2]

[1]*IMDEA Nanociencia, Madrid, Spain*
[2]*Departamento de Química, Universidad Autónoma de Madrid, Madrid, Spain*
Contact Email: marc.alias@imdea.org

In the last decades, the apparition of time-resolved pump-probe experiments has allowed us a deeper understanding on the photochemical processes. The development of new techniques has provided ultrafast temporal resolutions, in the attosecond scale, that may catch the electronic motion. Despite that fact, the interpretation of the time-resolved spectra is far from trivial and a strong theoretical support is a must to move further and achieve the desired goals. The use of an attosecond pulse in a molecule generates a coherent superposition of states because of its large bandwidth. These initial coherences evolve on time tending to disappear for the nuclear motion, but they also may revive or live longer times depending on the potential energy surfaces of the excited states. In the current study, we have analysed the evolution of coherences in LiH using different laser pulses through nuclear quantum dynamics using Multi-Configuration Time-Dependent (MCTDH) method.

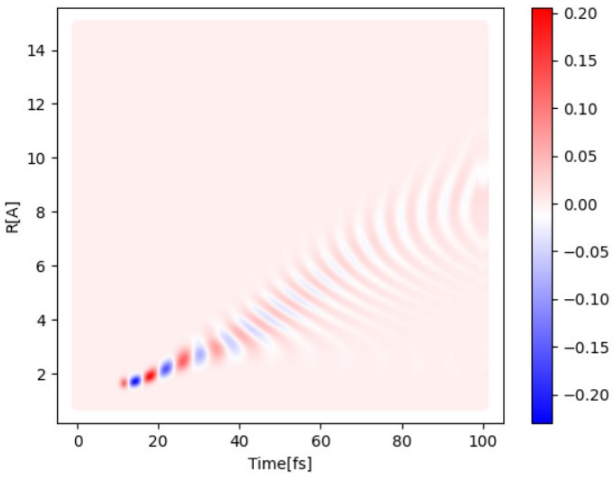

Figure 1: Real part of Σ_2-Σ_4 coherence along space and time