

Seminario de Química Física



Miércoles 11 de diciembre de 2024 – 11:30 h



Salón de Actos de la Biblioteca

Dr. Sandra Gómez

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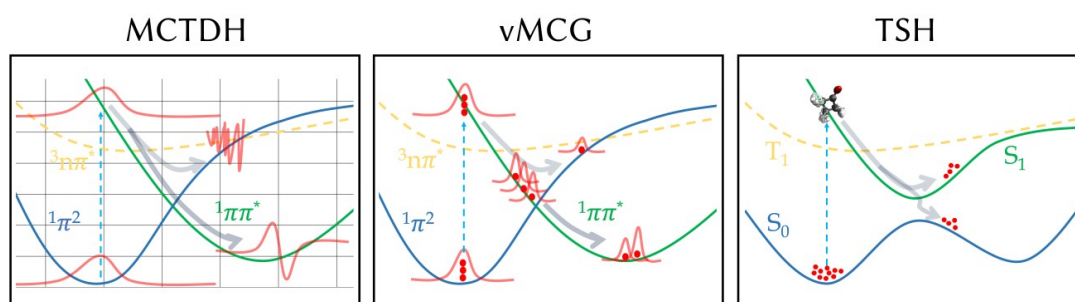
Universidad Autónoma de Madrid, Madrid E-28049



Navigating nonadiabatic dynamics methods for photoexcited molecular systems

Understanding how molecules respond and evolve after absorbing light is crucial for many areas of science. This complex process requires methods known as nonadiabatic molecular dynamics, which model molecular motion across multiple interacting energy levels. These techniques allow researchers to capture the intricate behavior of nuclear wavepackets as they move, split, and recombine across energy surfaces. With a range of approaches available—each built on distinct assumptions—selecting the appropriate method for a given scenario presents an ongoing challenge in this evolving field.

In this seminar, I will introduce three main methods: a precise grid-based method, a method in which the nuclear wavepacket is represented as a sum of fixed Gaussians, and the widely used surface hopping method, where independent nuclear structures are propagated and collected with the aim of approximating true wavepacket evolution. To illustrate, I will present examples from recent studies where we applied these methods to specific molecules, explaining why each was chosen[1-2]. I will also highlight the importance of reliable benchmarks for evaluating these techniques[3], especially as this field—still very young—continues to grow. Additionally, I'll showcase the **Quantics program package**[4], which enables these different methods to be tested on the same energy surfaces, making comparisons and benchmarks easier. The seminar will end with a look at potential future research directions and collaboration opportunities.



[1] Alberto Martín Santa Daría, Lola González-Sánchez, and Sandra Gómez, *Phys. Chem. Chem. Phys.*, 2024, **26**, 174-184.

[2] Alberto Martín Santa Daría, Javier Hernández-Rodríguez, Lea M. Ibele, and Sandra Gómez, *J. Chem. Phys.*, 2024, **160**, 114303.

[3] Sandra Gómez, K. Eryn Spinlove, and Graham Worth, *Phys. Chem. Chem. Phys.*, 2024, **26**, 1829-1844.

[4] M. H. Beck, A. Jäckle, Graham Worth, and Hans-Dieter Meyer, *Phys. Rep.*, 2000, **324**, 1.