Contribution ID: **25** Type: **Contributed talk**

# The Importance of Being a Conical Intersection in Ultrafast Photochemistry

*Monday, June 23, 2025 5:20 PM (20 minutes)*

It is well accepted that the most general case of photoinduced reaction dynamics occurs through non-adiabatic transitions. The complex panorama of potential energy surfaces describing the excited states of polyatomic molecules is characterized by non-adiabatic crossings and the presence of multiple conical intersections. A conical intersection (CI) is a 3N-8-dimension hypersurface of intersection between two electronic states. The two remaining internal coordinates, i.e., g as the difference gradient vector, and h as the non-adiabatic coupling vector, define the branching plane. Conical intersections can be considered as the transition states of electronic excited states and therefore the coupling between the different degrees of freedom, valence electrons and vibrations, and the timescales of these motions, are at the heart of the understanding of photochemistry. The main aim is to find an equivalent of the “Polanyi rules”for excited state polyatomic dynamics, in such a way that specific vibrational dynamics at CIs would be as important to dynamics as are the topographical features of the CIs themselves. In this contribution, we will highlight several cases of ultrafast non-adiabatic reaction dynamics in which CIs play a determining role for the photoinduced dynamics in ultrafast timescales. We will focus on the non-adiabatic dynamics in vinyl iodide [1] and the methyl iodide cation [2].

[1] M. L. Murillo-Sánchez, S. Marggi Poullain, P. Limão-Vieira, A. Zanchet, N. de Oliveira, J. González-Vázquez, Luis Bañares, Phys. Chem. Chem. Phys., submitted (2025).
[2] J. González-Vázquez, G. A. García, D. V. Chicharro, S. Marggi Poullain, L. Bañares, Chem. Sci. 15, 3203(2024).

**Author:** Prof. BAÑARES, Luis (Universidad Complutense de Madrid)

**Presenter:** Prof. BAÑARES, Luis (Universidad Complutense de Madrid)

**Session Classification:** Session 4 - Theory