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Tutorial: Excited-state dynamics

Wednesday 16 August 2023 08:00 (2 hours)

Photoinduced processes play a crucial role in different fields of science, for example, the photoisomerization of the retinal chromophore or the synthesis of vitamin D3. Additionally, they are crucial in the development of new technologies such as molecular electronic devices which can be controlled by light. These processes are governed mainly by nonadiabatic transitions which are radiationless electronic transitions between different non-Born-Oppenheimer states along the dynamic of a chemical reaction. In these two lessons, we are going to implement the Tully algorithm in Python to study a simple avoid crossing model as the first approach to a non-adiabatic transition.

Presenter: SALAZAR, Edison (U Groningen)