Contribution ID: **112** Type: **Contributed talk**

The Excited State Dynamics of Ethylene: A new theoretical model

Monday, June 23, 2025 11:50 AM (20 minutes)

The excited state dynamics of ethylene following excitation into the energetically lowest lying absorption band, nominally understood as arising from the $\pi\pi^*$ and $\pi 3s$ states, have been the focus of numerous theoretical and computational studies for many decades. Here, we present new quantum dynamics computations and spectroscopic simulations that indicate the non-adiabatic population dynamics can be better understood as arising from strong vibronic coupling between the $\sigma\pi^*$ and $\pi\pi^*$, and separately, between the $\sigma 3s$ and $\pi 3s$ electronic states. This model is shown to offer a clear explanation for previously unassigned bands in the UV absorption spectrum and is the basis for the interpretation of recent time-resolved photo-electron spectrosopic results.

Author: SCHUURMAN, Michael (National Research Council of Canada)

Co-authors: Dr JOUYBARI, Martha (University of Ottawa); Dr NEVILLE, Simon (National Research Council of Canada)

Presenter: SCHUURMAN, Michael (National Research Council of Canada)

Session Classification: Session 2 - Gas Phase Dynamics