

Poster: Individual and Collective Nonadiabaticity in Cavities

Full-dimensional quantum-dynamical simulations of homonuclear diatomic molecules inside Fabry-Pérot cavities are performed. Accompanied by analytical results, conical intersections (CIs) between polaritons are identified whose branching spaces are spanned by molecular rotations inside the cavity polarization plane. They are closely related to light-induced CIs (LICIs). However, unlike LICIs, they are of collective nature since they depend on the relative orientation of molecular electronic transition dipoles. We demonstrate numerically that, in the collective regime, ultrafast rotational dynamics around both types of CIs are coexistent, adding to the complex interplay among molecular structure and photonic modes in gas-phase cavity chemistry. Such rotational dynamics depends critically on light-molecule coherence which can be exploited to probe nonradiative decay towards the dark state manifold.

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