Dynamics of fulvene excited state with MCTDH (Multiconfiguration Time-dependent Hartree)

Lluís Blancafort, IQC, Jan 27th 2010

The presentation will focus on the non-adiabatic quantum dynamics of fulvene in its excited state carried out with the MCTDH method, in collaboration with H.-D. Mayer (Univ. Heidelberg, Germany). The photochemical process under study is a model double bond isomerization in the excited state that competes with the unreactive decay to the ground state, and the competition is related with a seam of intersection between the ground and excited states. The results include the parametrization of a 4-dimensional surface for the dynamics, and first dynamics results.