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Insights into the nonadiabatic dynamics of radical cations

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The fate of molecular systems when they interact with photons is almost always affected by nonadiabatic processes. Conical intersections between two or more electronic states are often present playing a crucial role in the dynamics. In this talk we focus on the importance of nonadiabatic effects in radical cations formed during photoionization. Motivation for this work has been the importance of the dynamics of radical cations in interpreting pump-probe experiments. Using surface hopping molecular dynamics and the Multi-Configurational Time-Dependent Hartree (MCTDH) approach we have studied the relaxation of several radical cations initially prepared in excited ionic states. We have found that radiationless decay to the lowest ionic state occurs very fast, and the direction of the derivative coupling plays an important role in the efficiency of the decay.