CALCULATION AND VISUALIZATION OF THE VIBRONIC EIGENFUNCTIONS OF JAHN-TELLER ACTIVE MOLECULES

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Jahn Teller active molecules are a convenient tool for understanding various nonadiabatic effects due to a conical intersection in the potential energy surface (PES), whether its position is determined by symmetry or accidentally along a reaction path. Computing PES, including the nonadiabatic coupling parameters, helps us to interpret the vibronic spectra of these molecules. Vibronic eigenfunctions are calculable either by utilizing fit data obtained from these vibronic spectra or electronic structure methods. In this talk we discuss the application and efficacy of these eigenvectors for calculating rovibronic parameters that characterize eigenstates in Jahn-Teller active molecules. Methods have been developed to plot spin vibronic eigenfunctions for multimode calculations. These plots give us considerable insight and enhance our understanding by visualizing Jahn-Teller interactions, multimode effects, and potentially the dynamics around a conical intersection.