

Physical Chemistry Seminar

Tuesday,
April 19, 2011

11:00 a.m.

Room 1315
Chemistry Building

Molecular Dynamics Around a Conical Intersection The Vibrations of Methoxy



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Conical intersections have a profound influence on many dynamical events. In the region around a conical intersection, multiple potential energy surfaces interact, and the Born-Oppenheimer approximation is no longer valid. In this talk I describe our research on the large amplitude vibrational dynamics of methoxy (CH_3O). The observed, complex spectroscopy observed for this radical results from a conical intersection at the C_{3v} geometry. To motivate the essential role of the conical intersection on the dynamics, I present results for a model Hamiltonian consisting of two vibrational degrees of freedom and the coupling between them. The advantages of working in a diabatic representation for the electronic degrees of freedom is highlighted. The calculated spectra are understood in terms of the multiple timescales that arise as the initial wave packet passes through the conical intersection. This model Hamiltonian is extended to include a full-dimensional treatment of methoxy.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:15 p.m. in Room 8305f