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Dissociative Electron Attachment to Water: Treatment of $^2B_1$, $^2A_1$, and $^2B_2$ resonances DANIEL HAXTON, The University of California-Berkeley and Lawrence Berkeley National Lab, THOMAS RESCIGNO, Lawrence Berkeley National Lab, C. WILLIAM MCCURDY, Lawrence Berkely National Lab and the University of California-Berkeley and the University of California-Davis —
The computational treatment of dissociative electron attachment to gas-phase water via each of the three involved Feshbach resonances, of $^2B_1$, $^2A_1$, and $^2B_2$ symmetry, is discussed, and preliminary results are reported. The behavior of each of these resonances with respect to variations in the nuclear geometry is examined, and several interesting features are discussed. These features include the conical intersection between the $^2A_1$ and $^2B_2$ states and a seam of degeneracy between the $^2B_2$ Feshbach resonance and a $^2B_2$ shape resonance. Seams of degeneracy between metastable states may involve an interesting topology in which the two degenerate states are interchanged by adiabatic following around the seam. This topology is reflected in each of the two seams comprising the $^2A_1$ / $^2B_2$ conical intersection, as well as the $^2B_2$ shape-Feshbach degeneracy. It finds a parallel in the theory of "hidden crossings" of bound states at complex nuclear geometries. Preliminary results on dissociative attachment via the Renner-Teller coupled $^2B_1$ ($^2A''$) and $^2A_1$ ($1\,^2A'$) states, obtained using the Multi-Configuration Time-Dependent Hartree (MCTDH) method and a local treatment of the nuclear dynamics, are presented and compared to experiment.

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