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Dissociative Electron Attachment to H_2O and H_2S DANIEL HAXTON, University of California - Berkeley & Lawrence Berkeley Lab, THOMAS RESCIGNO, Lawrence Berkeley Lab, C. WILLIAM MCCURDY, University of California - Berkeley & Lawrence Berkeley Lab & University of California - Davis —
Dissociative electron attachment (DA) to H_2O is of direct importance for both biological and techological systems. The calculations on H_2O and H_2S presented comprise the first *ab initio* treatment of DA to a polyatomic molecule employing the full dimensionality of nuclear motion. Cross sections obtained for DA via the $^2B_1$ state of H_2O agree well with experiment, reproducing the high degree of vibrational excitation of the OH fragment. Several interesting features of the A' manifold of resonances for H_2O have been discovered, including a conical intersection between the $^2A_1$ and $^2B_2$ Feshbach resonances and a branch-point degeneracy between the $^2B_2$ shape and Feshbach resonances. This latter feature has no analogue in bound-state theory. We show results of recent calculations on the Renner-Teller coupled $^2A_1$ and $^2B_1$ surfaces, and on electronically coupled diabatic $^2A_1$ and $^2B_2$ surfaces. The angular dependence of the H^- + OH channel for the $^2B_1$ state of H_2O and that of the analagous channel and state of H_2S have been calculated by incorporating the mixing of different partial waves into the entrance amplitude, and for H_2S, the variation of this mixing with geometry.

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