Abstract Submitted
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Two- and three-body breakup in dissociative electron attachment to water D.J. HAXTON, JILA and the University of Colorado, Boulder, T.N. RESCIGNO, LBNL, C.W. MCCURDY, LBNL, UCB, UCDavis — We present calculations on two- and three-body breakup in dissociative electron attachment (DEA) to water,

$$e^- + H_2O \longrightarrow H^- + OH, H_2 + O^-, ...$$

This process is mediated by three metastable electronic states (Feshbach resonances) of H_2O^- which are coupled by a conical intersection and by Renner-Teller coupling. We define complex-valued potential energy curves using *ab initio* scattering and bound-state calculations. We use these coupled curves in calculations of the time-dependent nuclear dynamics using the Multi Configuration Time Dependent Hartree (MCTDH) approach. For DEA via the higher $^2A_1$ and $^2B_2$ Feshbach resonances, the three body channels are open. We discriminate between two- and three-body breakup in this system by performing calculations in both Jacobi and hyperspherical coordinate systems. We provide strong evidence that the observed O^- production from the $^2A_1$ resonance state is exclusively due to three-body breakup. For DEA via the highest $^2B_2$ state, our treatment of the dynamics is necessarily imperfect, but we achieve good agreement with experiment in certain respects. We explain how the conical intersection plays a crucial role in the nuclear dynamics.

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