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Nuclear dynamics of dissociative electron attachment to water via the conically intersecting $^2B_2$ and $^2A_1$ states[1] DANIEL HAXTON, THOMAS RESCIGNO, Lawrence Berkeley National Laboratory, C. WILLIAM MCCURDY, University of California, Davis and Lawrence Berkeley National Laboratory — We present theoretical results on the nuclear dynamics of dissociative electron attachment to the water molecule via the highest-energy $^2B_2$ electronic Feshbach resonance state of the anion. These results accompany the experimental results of Adaniya et al. The process in question is complex, involving a conical intersection of Born-Oppenheimer potential energy surfaces and several two-and three-body final fragment states. Surface-hopping classical trajectory calculations including the effect of autoionization are performed with previously calculated potential energy surfaces for the intersecting $^2B_2$ and $^2A_1$ states, and the amplitude for attachment as a function of nuclear geometry and incident angle of the electron in the molecular frame is also determined. This permits a reconstruction of the lab frame fragment angular distribution and the explanation of its features in terms of the multidimensional nuclear dynamics of the dissociation process.

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