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Double photoionization of H_2 using a hybrid Gaussian-discrete variable representation basis for molecular continuum processes¹ FRANK L. YIP, California State University-Maritime Academy, C. WILLIAM MCCURDY, UC Davis and Lawrence Berkeley National Lab, THOMAS N. RESCIGON, Lawrence Berkeley National Lab — A hybrid basis that combines Gaussian basis functions typically used in bound-state molecular electronic structure calculations with a grid-based discrete variable representation (DVR) suitable for continuum processes involving one or more electrons is used to fully describe the double ionization of molecular H_2 by a single photoabsorption. Comparison will be made with the most detailed information that has been calculated and measured for this Coulomb explosion: the triply differential cross sections that relate the angular distribution and energy sharing of all of the particles in the frame of the molecule. The advantages of utilizing this hybrid basis for double ionization processes beyond this simplest molecular target will be highlighted.

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