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First-Principles treatment of molecular double photoionization[1]
DANIEL A. HORNER, T.N. RESCIGNO, LBNL, C.W. MCCURDY, LBNL, UC Davis — We have developed a new computational approach to solving molecular double photoionization problems. The approach combines both Gaussian functions and the grid-based, exterior complex scaling discrete-variable representation (ECS-DVR) in a hybrid basis. Gaussian functions are well established and ideal for expanding molecular electronic states and the ECS-DVR on a finite-element grid has had much success solving atomic electron-impact ionization and double photoionization problems. The hybrid Gaussian ECS-DVR method allows us to extend our treatment of problems with two active electrons in the continuum to molecular targets. We have performed calculations of absolute fully-differential cross sections for the double photoionization of molecular hydrogen. Unlike other model calculations, this is a true *ab initio* approach.

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