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Single photon induced symmetry breaking of H_2 dissociation

THORSTEN WEBER ET AL., Lawrence Berkeley National Lab — Symmetries are essential building blocks of our physical, chemical and biological models. For macroscopic objects symmetries are always only approximate. By reducing the complexity in the microcosm these symmetries often become strict. In H_2 and H_2^+, the smallest and most abundant molecules in the universe, this complexity is reduced to the minimum. They have perfectly symmetric ground states. What does it take to break this symmetry? In our study we show how and why the inversion symmetry of the hydrogen molecule can be broken by absorption of a linearly polarized photon, which itself has inversion symmetry. The emission of an electron with subsequent dissociation of the remaining H_2^+ shows that under some circumstances no symmetry to the ionic and neutral fragment. This is the smallest and most fundamental molecular system for which such symmetry breaking is possible. The mechanisms identified behind this symmetry breaking are general for all molecules. Fully differential angular cross sections, which have been experimentally obtained with the COLTRIMS technique (using linear polarized light ranging from 32 to 50 eV at the Advanced Light Source) are compared with a state-of-the art quantum mechanical approach implementing B-spline basis sets.

Thorsten Weber
Lawrence Berkeley National Lab

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