SINGLE PHOTON INDUCED SYMMETRY BREAKING OF D_2 DISSOCIATION

Th. Weber[1], F. Martin[2], J. Fernandez[2], T. Havermeier[3], L. Foucar[3], K. Kreidi[3], M. Schoeffler[3], L. Schmidt[3], T. Jahnke[3], A.L. Landers[4], O. Jagutzki[3], A. Czasch[3], T. Osipov[1], A. Belkacem[1], M. H. Prior[1], H. Schmidt-Boecking[3], C.L. Cocke[5], and R. Doerner[3]

[1] Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA - [2] Departamento de Quimica, Universidad Autonoma de Madrid, Madrid, 28049, Spain - [3] Institut für Kernphysik, Universität Frankfurt, D 60486 Frankfurt, Germany - [4] 206 Allison Laboratory, Auburn University, AL 36849 5311, USA - [5] Dept. of Physics, Kansas State University, Manhattan, KS 66506, USA

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^+ respectively D_2 and D_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 ?

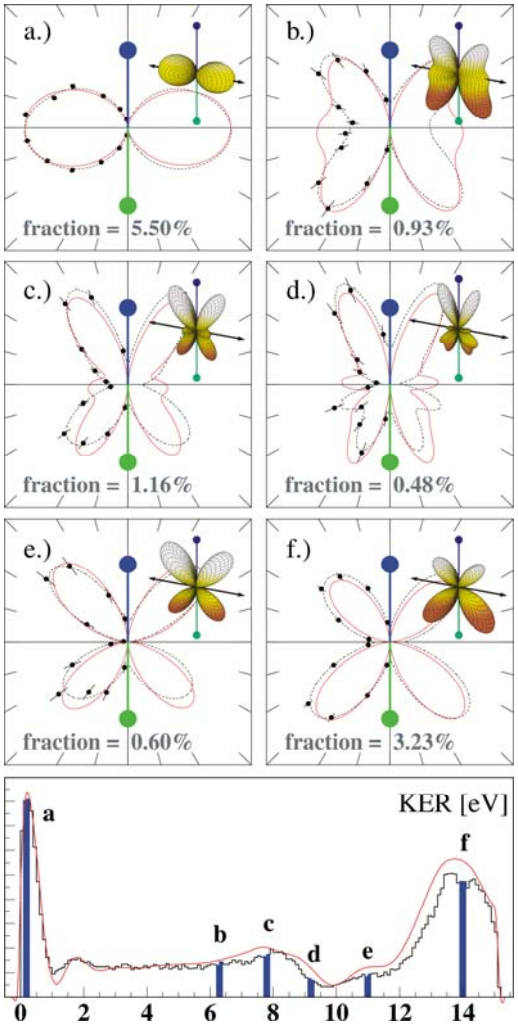

Fig 1. Fully differential angular cross sections (see text).

In our study [1] we show how and why the inversion symmetry of the hydrogen (respectively deuterium) 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 D_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 are compared with a state-of-the art quantum mechanical approach implementing B-spline basis sets:

Fig 1 shows the angular distribution of the electrons as a function of KER for dissociative ionization of D_2 at a photon energy of 33.25 eV, linearly polarized light. The orientation of the molecule at 90° to the polarization (theory) and 90° ± 10° (experiment) is indicated by colored circles (blue, deuteron; green, deuterium). The (horizontal) polarization vector and the molecular axis define a common plane. The electron is restricted to this plane by ±45°. Solid red line, theory; circles with error bars (where error is SD), experiment; dotted line, fit of the experimental data with spherical harmonics. The theoretical results have been integrated over the experimental acceptance angles and KER resolution as well as electron resolution. Infinite resolution theoretical results are shown by the small threedimensional plots in the upper right: KER = 0.2 (a), 6.3 (b), 7.8 (c), 9.2 (d), 11 (e), and 14 eV (f). Units are arbitrary units. (B) The angle integrated KER spectrum. Red line, theory; black line, experiment; letters a to f correspond to a to f in (A); KER intervals are ±0.1 eV. The x-axis shows KER in eV. The y-axis shows a cross-section in arbitrary units.

References:

[1] F. Martín et al., Science 315, (2007), 629