Research Training Group 2721
Hydrogen Isotopes ^{1,2,3}H
P1 / Prof. Knut Asmis

UNIVERSITÄT LEIPZIG

Fakultät für Chemie und Mineralogie
Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie

Focused Lecture

Prof. Evan Bieske

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Monday, 28 August 2023 / 2:30 – 3:30 pm CEST

Kl. HS / room 015 – Johannisallee 29 – 04103 Leipzig

Spectroscopically probing interactions of H_2, D_2 and HD with halide anions and metal cations – a molecular view of hydrogen storage

The storage of molecular hydrogen in solid media (zeolites and MOFs) often depends on the interactions of H_2 and metal cations or halide anions. To better understand the operative interactions we have spectroscopically probed a series of complexes in the gas phase. Target species include H_2 and D_2 attached to the Cl^-, Br^-, I^- anions, and to the Li^+, Na^+, B^+, Al^+, Mg^+, Mn^+, Zn^+ cations. The infrared action spectra exhibit rotational resolution and deliver fundamental insights into the intermolecular interactions. The anion complexes (Cl^-–H_2, Br^-–H_2, I^-–H_2 *etc.*) are linear, whereas the cation complexes (Li^+–H_2, Na^+–H_2, B^+–H_2 *etc.*) are T-shaped, consistent with the dominant charge-quadrupole interactions between the ion and the H_2 molecule. There are several notable features of the spectra. First, it is apparent that *ortho* H_2 is bound more strongly than *para* H_2 to both the anions and the cations. Second, the systems are highly quantum in nature and undergo large amplitude vibrational motions with the Cl^-–H_2, Br^-–H_2 and I^-–H_2 spectra showing clear signs for tunnelling splitting associated with internal rotation of the D_2 sub-unit. In some cases, such as Cr^+–D_2, the onset of dissociation at a particular excited rovibrational level allows us to place narrow bounds on the dissociation energy, providing a solid benchmark against which current computational techniques can be measured.

The lecture will be streamed via Zoom:

https://uni-leipzig.zoom.us/j/67221664393?pwd=eFRVRm5URE9rc256WDh3ZTB3NnNlZz09

Meeting ID: 672 2166 4393 / Passcode: 245588