From Dihydrogen Bonded Systems to Hydrogen Storage Materials

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The nature of dihydrogen bonded (DHB) system has been studied in out lab in last years, with a final conclusion that it is very similar to that of regular hydrogen bonds. By using different tools, it was shown that they are provided by roughly 40-60% of orbital interaction energy, with topological description not far from the hydrogen bonded-systems.

From previous studies it was shown that there are a qualitative differences between donor-acceptor DHB and H_2 formation. This clear-cut difference can, however, turn into a more gradually changing spectrum in asymmetric model systems AH···HX that feature hydric and protonic hydrogen atoms. This analysis suggested a design principle for hydrogen storage materials. Thus, by varying the electronegativity difference between H and X in H–X (but also between A and H in AH), one can tune the stability or lability of the DHB system towards conservation or elimination of the central H_2 unit. The objective is then to arrive at a material that undergoes thermoneutral uptake and release of molecular hydrogen via a low activation barrier.

This talk will be focused in different systems that can be used as hydrogen storage materials. Using different substituents one can modulate the activation barrier as well as the total reaction energy.