

## Investigation of supramolecular bonding

(Kyoto University, Dep. Of Microengineering\*, Wroclaw University of Technology, Chemistry Dep.\*\*)  
 ○ Pawel Szarek<sup>\*,\*\*</sup>, Akitomo Tachibana<sup>\*</sup>, Andrzej W. Sokalski<sup>\*\*</sup>

The supramolecular creation is often provided by the hydrogen bonding (h-bonding, for short). This particular interaction between two electronegative atoms bridged by a proton in small systems is being reviewed here using Rigged QED theory [1] and non-empirical variation-perturbation decomposition of interaction energy [2]. The geometry and the distance on electronic stress and on interaction energy have been investigated. The comparison with ionic, covalent and non-bounded systems allows estimating the nature of hydrogen bonding in studied cases. This intermolecular interaction arises from the balance of several components: long range electrostatics, induction and dispersion, or overlap (size repulsion and charge transfer) at short distances. Charge sheering indicates covalent character of h-bonding interaction as well as cooperative effects caused by charge flow [3]. On the other hand strong polarization of interacting species indicates the electrostatic origin of interaction effects.

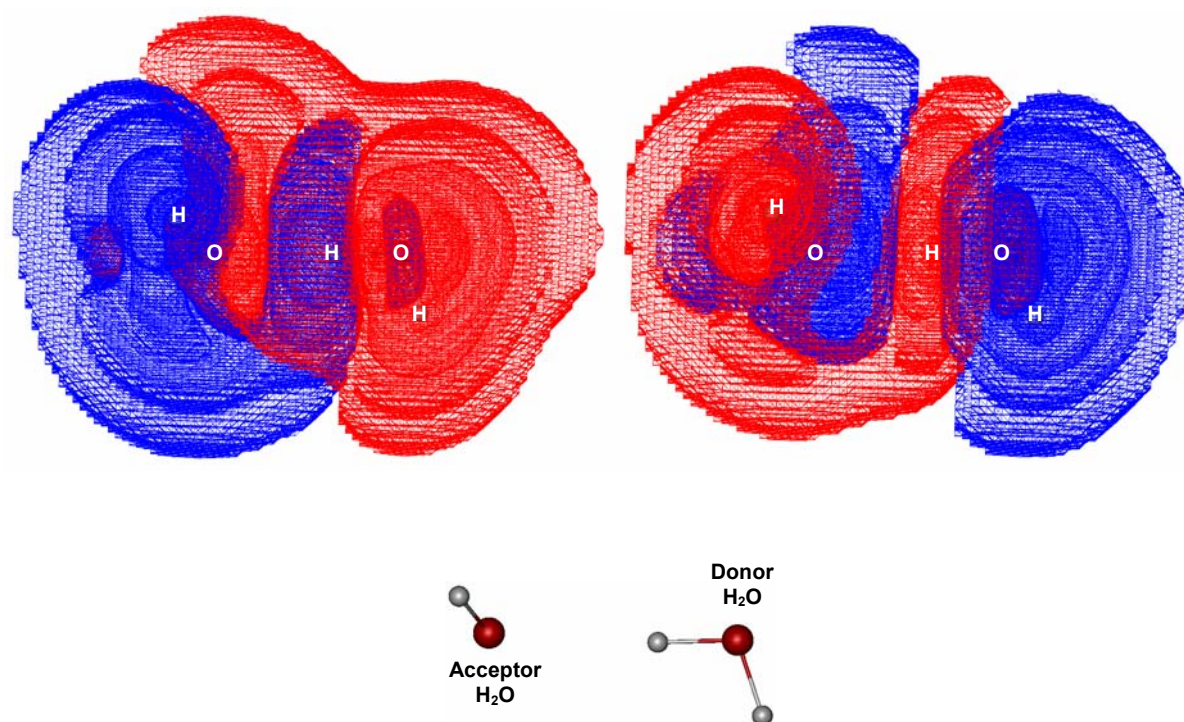


Figure 1. Hydrogen bond in water dimer: a) electron density change in system as a difference of dimer electron density and densities of monomers; blue corresponds to regions of decreased electron density (hydrogen atoms of acceptor water molecule and bridging proton), while red indicates increase of electron density (lone pairs of oxygen atoms and O-H bond between donating O atom and bridging H atom); b) Stabilization Energy Density; blue areas denote local stabilization and red – local destabilization of bonding interaction; destabilization is mainly caused by withdraw of electrons from the local area.

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