Hydrogen bonds explained by Kohn-Sham Molecular Orbital Theory

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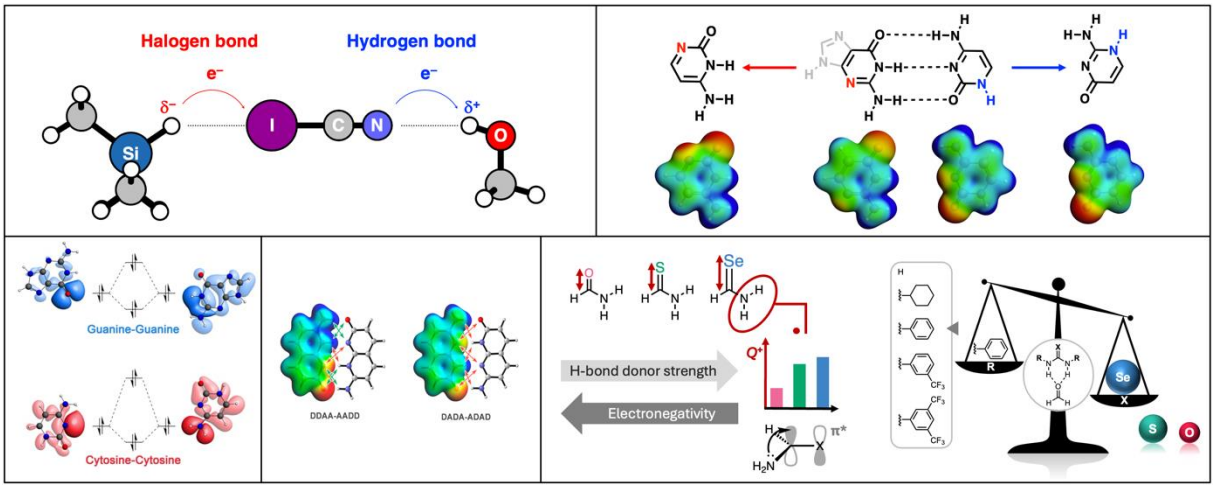
Hydrogen bonds are omnipresent in biological and supramolecular chemistry. Nevertheless, they are still mostly represented in an oversimplified manner which is easy to use but often fails to explain or even qualitatively reproduce experimental findings. In my lecture, I present a state-of-the art physical model, based on quantitative molecular orbital theory, which enables a quantum-mechanically sound, yet intuitive approach to the interesting complexity of the hydrogen bond. The latter can be dissected into understandable contributions such as electrostatic interactions, covalent bonding and Pauli repulsion between occupied orbitals. Complex and seemingly exotic phenomena are unraveled and explained in a unified manner: definition of hydrogen bonding, [1,2] role of aromaticity in hydrogen bonds,[3-6] variations in hydrogen bond lengths and energies due to steric repulsion,[7] legitimacy of the secondary electrostatic interaction model[8] and hydrogen bond donor capability of carboxamides, thioamides and selenoamides.[9-11]



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