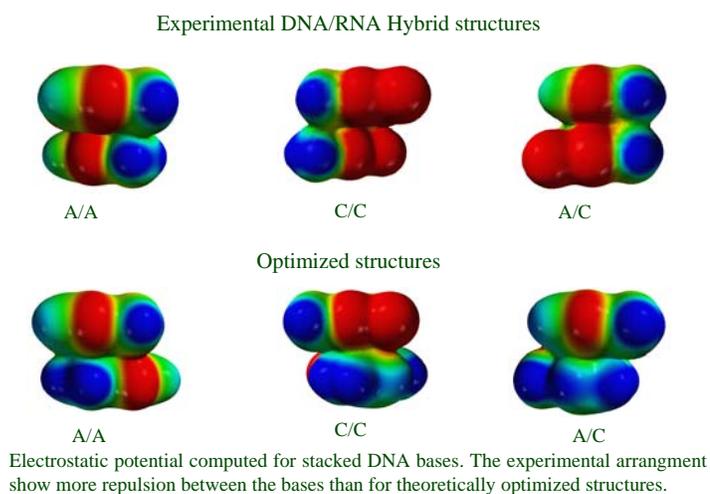


Theoretical Studies of The Interplay between Non Covalent Interactions in Biomolecules and of The Basicity of Zeolites.

In a first part, we will see the influence of the stacking interaction on the ability of aromatic compounds to form hydrogen bonds. Various stacked complexes are studied comprising stacking aromatic molecules (benzenes) substituted with electron donating/withdrawing groups. The hydrogen bonding acceptor/donor aromatic molecules are pyridine, pyrimidine, histidine, tyrosine and DNA bases. Different orientations of the stacking molecules are investigated. The intrinsic properties of the stacking molecules, such as the hardness, and the hydrogen bonding ability of the stacked molecule in the complex are also related and correlated to the interaction energy contributions, in particular the electrostatic interaction, and to the charge transfer between the stacked molecules.

It was found that the hydrogen bonding ability was related to the global hardness of the substituted benzenes. Also an inverse correlation between the electrostatic interaction and the hydrogen bonding ability of pyridine was observed. The role played by the orientation of the stacked showed that parallel stacking leads to a larger hydrogen bonding ability than T-shaped stacking. The local hardness appeared to be the key index linking the electrostatic interaction to the hydrogen bonding ability of the base. Finally, these findings were extended to stacked DNA bases.



In a second part DFT based reactivity descriptors are tested for their ability to describe the basicity of Al-O-Si bridging oxygen in alkaline cation exchanged zeolite. In a first study of the methylation reaction of bridging oxygen by methanol and methyl iodide, we tried to discern the effect/influence of the Lewis acidity of the alkaline cation and of the oxygen basicity. Also the Electrostatic potential is proposed as a good descriptor of basicity. Secondly the electrostatic potential and the local hardness are tested for their ability to reproduce the variation of the oxygen basicity for different alkaline cations and different isomorphous substitutions. These results are also compared with the proton affinity and with the adsorption energy of NO^+ .