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Non-covalent interactions and their role in chemistry and biosciences

Noncovalent interactions play a key role in chemistry and biosciences and they are responsible for structure of water and biomacromolecules. It should be mentioned that function of biomacromolecules is to large extent determined by their structure - e.g. the doublehelical structure of DNA is responsible for storage and transfer of genetic information. Experimental study of noncovalent interactions is difficult and not unambiguous. On the other hand theoretical procedures of quantum chemistry combined with methods of molecular dynamics provide a unique and consistent picture of noncovalent interactions in different environments as well as at different temperatures. In the lecture different types of noncovalent interactions will be mentioned together with their nature and the role they play in nature. Further, computation methods will be discussed, starting from the most accurate, nonempirical ones providing the chemical or even spectroscopical accuracy up to semiempirical and empirical ones allowing to study systems with several thousand of atoms. Finally, selected projects from our laboratory will be briefly mentioned and attention will be paid to in silico drug design.