Theoretical Chemistry: Noncovalent Interactions in Molecules and on Surfaces

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Last century, the nature of strong interactions between atoms, being responsible for configuration and conformation of molecules, were in the focus of chemical research activities. Nowadays, in modern quantum chemistry, such strong interactions are rather well understood and became an indispensable tool for all fields of chemistry. However, the description of weak interactions between atoms and molecules, which are responsible for the characteristics of the solid and liquid state, mostly remain unsolved and therefore attract considerable attention.

In recent years, theoretical chemistry has contributed efficiently to the desired knowledge, as demonstrated by the rapidly increasing number of papers in computational chemistry on the topic of non-covalent and intermolecular interactions. Various methods are available for computations, whereas the development, assessment and combinations of these methods are in the center of this presentation. The computational applications are manifold. Here, we focus on intermolecular interactions between molecules [1-6] and molecular arrangements on surfaces [7-8].

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