

State-of-the-art and perspectives in modeling of London dispersion forces

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With the rapidly increasing computational power the sub-chemical level of accuracy determination of energy differences is within the reach of theoretical chemistry. This development has given a soaring rise of studies on weak intermolecular – van der Waals – forces, in particular on London dispersion interactions. The considerable importance of these universal attractive forces cannot be overestimated in chemistry, physics and biology. It has been shown on numerous examples that, in contrast to earlier ideas, London dispersion forces play an essential, sometimes decisive rôle in the understanding of the structure and energetics, not only of intermolecular complexes but also in many other situations.

The purpose of this talk is to give a broad overview of the most important wave function and density functional approximation methods, which are appropriate for a quantitative description of dispersion interactions. Different hybrid procedures have been designed to correct the failure of common density functional approximations. Special attention will be paid to the Random Phase Approximation (RPA), which gained a considerable popularity in recent years, and seems to provide a sound basis for the discussion of some conceptually interesting phenomena like different types of the non-additivity, which can be manifested in different ways.