

A computational method for description of the intermolecular interactions in excited states.

Covalent bonds are responsible for the molecular form of water, oxygen and other substances in nature. Apart from those there exist the non-covalent interactions, which are weaker than the covalent ones, but equally as important. They are the reason behind the existence of different phases of matter, they facilitate or impede certain chemical reactions and they define the spatial structure of molecules.

The description of those interactions, because of their subtlety, is often difficult for theoretical chemists, but it is essential for accurate modelling of materials and chemical reactions.

The most popular group of computational methods – DFT – initially was not able to describe the noncovalent interactions, but thanks to introducing special corrections is now able to do this. Unfortunately those corrections have only been introduced for the ground state. This means that when a molecule of interest absorbs some light, we are no longer able to describe its interactions with the environment. This is not ideal, since the excited matter is very interesting for chemists, physicists and engineers.

In particular, modelling of materials for solar cells and molecular photoswitches requires a good description of both excited states and of noncovalent interactions. The solar cells transform the energy in a light form into electrical one. They are currently the best chance of substituting carbon as the main source of the electrical energy. The photoswitches are molecules that change their structure in response to light, which e.g. allows them to open or close a nanoscale electrical circuit. If we could find the best possible candidate molecules for solar cells and photoswitches, we would significantly lower the cost of their production – instead of having to obtain and then test tens or hundreds of molecules, it would suffice to model them on a PC and then only create in a lab a few best candidates.

This project's goal is to fill the gap in the computational chemistry's toolbox and developing a method that would describe efficiently and accurately the noncovalent interactions in the excited state. The method will be implemented in a popular package for quantum-chemical computations and then employed for describing systems like perylene and its derivatives, with applications in solar cells, which can help build more efficient solar cells in the future.

The main result of the project will however be the method itself which, as the first DFT method in the world will be able to describe the noncovalent interactions in the excited state.