DESCRIPTION FOR THE GENERAL PUBLIC

Hydrogen atom – the simplest and lightest element – takes part in many basic chemical reactions. Among those, the most popular are the processes in which a proton, i.e., hydrogen atom devoid of the electron, detaches from a molecule called the acid and attaches to a molecule called the base. The mechanism of this seemingly simple reaction is still not completely understood, because of the role played by quantum effects, the phenomena unknown in classical physics and chemistry. The observation and correct description of such effects remain the challenges for both experiment and theory.

Hydrogen atom can migrate not necessarily between different molecules. An intramolecular reaction is also possible. This phenomenon is called tautomerization, and the forms of the same molecule that differ in the location of the proton are called tautomers. Among all the possible tautomers, one usually has the lowest energy and is therefore the only one or a dominant species observed.

The goal of the proposed investigations is to obtain and observe rare tautomeric forms, which, albeit theoretically possible, have not been detected so far because of too high energy. Our previous investigations have demonstrated that such species can be obtained if a molecule is placed on the surface of a metal crystal, e.g., on copper or silver. Under such conditions, the relative energies of the tautomers can change in such a way that the form normally not observed becomes the most stable.

The objects of our studies will include molecules related to porphyrin, called “pigment of life”, because of its crucial role in such processes as photosynthesis or oxygen transport in blood. Knowing the properties of rare tautomeric form will help in the detailed understanding of the tautomerization mechanisms. Such knowledge may be utilized in practice for creating molecular switches or memories of which the operation principle is based on controlled interconversion between the tautomeric forms.