Theoretical studies of selected hydrogen bonded systems will be performed by theoretical methods in the ground and excited electronic states. These studies will include high precision ab initio quantum chemical calculations performed to obtain information on energies, structures, and spectral parameters of investigated compounds.

This project includes quantum-mechanical calculations and interpretation of infrared and Raman spectra of hydrogen-bonded systems, theoretical study of photophysics of purine-pyrimidine dimers, present in nucleic acids, calculations ising molecular dynamic methods and study of proton tunneling in hydrogen-bonded systems.

The aim of these studies is to understand the nature of hydrogen bonds and proton tunneling.