To the world of inter- and intramolecular interactions I have recently introduced a new type of interaction that can be formally labelled as Xδ+-Hδ-···>Y. Interaction of this type was coined a term charge-inverted hydrogen bond (CIHB) due to the opposite 'polarization' in the X-H···Y bridge as compared to a hydrogen bond. On the basis of formal definitions of diverse intermolecular interactions possessing a hydridic hydrogen atom (dihydrogen bond, hydride hydrogen bond, agostic bond, etc.) as well as on the basis of results obtained by means of QTAIM and HVPT calculations I have very recently shown that CIHB should indeed be investigated as a new type of interaction. Further studies on differences between agostic bond and CIHB are being planned. So far I have characterized four R3XHδ-···>YZ3 dimers with CIHB. The aim of the present project is to considerably increase the amount of known systems with CIHB by those involving chosen X and Y atoms as well as some R and Z substituents. This idea is to further inspire some other scientists to experimentally confirm the existence of CIHB. That is also why we are going to perform high level (i.e. state-of-the-art) calculations of experimentally measurable structural and spectroscopic parameters referring to the charge-inverted hydrogen bond. The present project is also aimed to significantly enlarge the knowledge of both the nature of CIHB as well as of properties of systems with CIHB.

Due to the fact that the charge-inverted hydrogen bond (CIHB) has been proposed only relatively recently and then it has been shown to represent a new type of interaction, each successive studies of systems with CIHB will include new cognitive elements and thus they will be pioneer. As such, they will be performed for the first time in the world. The proposed studies will significantly broaden the scope of knowledge of the nature of the charge-inverted hydrogen bond as well as of properties of systems with CIHB. Simultaneously, the increase of the number of theoretically studied systems with CIHB and the calculation of exact values of experimentally measurable structural and spectroscopic parameters should encourage other scientists to experimentally confirm the existence of CIHB. This knowledge can greatly facilitate the collection of experimental data concerning systems with CIHB in gas phase and in matrices of noble atoms. Studies of the influence of the type of X, Y, R i Z on the strength of a complex should have a significant impact in e.g. material engineering. Further studies of the differences between CIHBs and agostic bonds will help to properly classify interactions and may strengthen the autonomy of CIHBs.

Calculations will be performed by means of DFT, MP2, and CCSD(T) methods. In the case of DFT we are going to use several exchange-correlation energy functionals, including also the newest ones that take into account corrections for dispersion. This may be particularly important in systems with bulky organic substituents. All calculations are planned to be performed by means of Gaussian09 suit of codes. More detailed studies of electronic structure are planned to be performed by means of AIMAll and NBO6.0 programs.