Reg. No: 2017/25/B/ST4/01024; Principal Investigator: prof. dr hab. Jacek Komasa

Fast development of the contemporary spectroscopic techniques enables the dissociation and transition energy of hydrogen molecule to be determined with precision exceeding 10^{-4} cm⁻¹. This fact imposes a necessity of increasing the accuracy of theoretical methods as well. Within this project we are going to apply a new accurate method of solving the Schrödinger equation. This method allows the nonrelativistic dissociation energy of rovibrational levels of H₂ to be determined with unprecedented accuracy of 10^{-7} cm⁻¹. Application of this approach to all bound levels of different isotopomers molecular hydrogen will results in a complete set of benchmark quality data base.

Reaching this project's goal will, in combination with increasingly accurate experimental data, open a route for increasing the precision of fundamental constants like the electron mass, Rydberg constant, or support the solution of the proton size puzzle. It will also enable tightening the bounds on the hypothetical fifth-force.

At present, the accuracy of the theoretical value for the dissociation energy of the ground level of H_2 is restricted mainly by the lack of the relativistic nuclear recoil contribution and the limited accuracy of the leading QED correction. Equipped with the nonadiabatic wave functions generated in frames of this project, we will be able to take into account also the finite nuclear mass effects in the relativistic and QED correction and eliminate this limitation. These wave functions will be used in future applications to determine with high accuracy also other (e.g. electric and magnetic) molecular properties.