Contribution ID: **70**   Type: **oral with proceeding**

Accurate calculations with explicitly correlated functions for molecular hydrogen

Wednesday 16 May 2018 11:05 (30 minutes)

Theoretical studies of hydrogen molecule is the cornerstone of the molecular quantum mechanics. Due to its simplicity, the achieved precision is the highest among all molecules and still has a potential of significant enhancement. This high precision of theoretical predictions for H_2 leads to improved tests of quantum electro-dynamics (QED) and improved bounds on hypothetical interactions. Moreover, at the 10^{-7} cm^{-1} precision level the dissociation energy is sensitive to the proton charge radius, which may help to resolve the so called proton radius conundrum. This requires high accuracy calculations of not only nonrelativistic energies, but also leading relativistic and QED, as well as the higher order QED corrections. In fact, the nonrelativistic energies can already be calculated with the precision of 10^{-7} cm^{-1}. The the higher order QED contribution has very recently been calculated using explicitly correlated Gaussian (ECG) functions with $1 + r_{12}/2$ prefactor ({\it rECG}) that makes the interelectronic cusp condition to be exactly satisfied. We provided improved results for the dissociation and the fundamental vibrational energies. These results open the window for the high precision spectroscopy of H_2 and related accurate tests of fundamental interactions models. Recently, we also reported also highly accurate results for the leading relativistic correction using {\it rECG} functions and conclude that the compilation of previous results has underestimated uncertainties. We will also present the latest advances in the calculation of nuclear mass relativistic corrections, which are currently the main limitation of theoretical predictions.

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Author: Prof. PUCHALSKI, Mariusz (Faculty of Chemistry, Adam Mickiewicz University, Poland)

Presenter: Prof. PUCHALSKI, Mariusz (Faculty of Chemistry, Adam Mickiewicz University, Poland)

Session Classification: Molecules #1