Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Nonadiabatic calculations on hydrogen molecule JACEK KOMASA, Adam Mickiewicz University, Poznan, KRZYSZTOF PACHUCKI, Warsaw University, Poland — Since its infancy quantum mechanics has treated hydrogen molecule as a test bed. Contemporary spectroscopy is able to supply the dissociation energy (D_0) of H_2 with the accuracy of $3.7 \cdot 10^{-4}$ cm^{-1}, while current theoretical predictions are 10^{-3} cm^{-1} in error. Both the uncertainties are already smaller than the quantum electrodynamic (QED) effects contributing to D_0, which poses a particular challenge to theoreticians. Undoubtedly, in order to increase the predictive power of theory one has to not only account for the multitude of the tiny relativistic and QED effects but, especially, significantly increase precision of the largest component of D_0—the nonrelativistic contribution. We approach the problem of solving the Schroedinger equation, equipped with new methodology, with the target precision of D_0 set at the level of 10^{-7} cm^{-1}.

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Date submitted: 06 Nov 2015 Electronic form version 1.4