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High-precision calculations of hydrogen molecule

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Highly accurate excited state energies in H2 provide a reliable method for determination of its ionization energy. We present H2SOLV - our numerical package capable of high-precision calculations of Σ and Π bound states of H2. Based on efficient method for calculations of two-center two-electron integrals with wavefunction represented as a linear combination of explicitly correlated exponential (Ko{\l}os-Wolniewicz) functions, it allows for multithreaded, large-scale computations limited only by the computer resources available and can produce highly accurate results.

We present results of exemplary application of our computational method for obtaining accurate Born-Oppenheimer energies, as well as dynamic polarizability calculations for different hydrogen isotopologues and to variational calculations of splitting energy between the lowest states of H2 for studies of long-range asymptotics of exchange energy.

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