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Including nuclear quantum effects into highly correlated electronic structure calculations of weakly bound systems

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Streszczenie

An interface between the APMO code and the electronic structure package MOLPRO is presented. The any particle molecular orbital APMO code [González et al., Int. J. Quantum Chem. 108, 1742 (2008)] implements the model where electrons and light nuclei are treated simultaneously at Hartree-Fock or second-order Möller-Plesset levels of theory. The APMO-MOLPRO interface allows to include high-level electronic correlation as implemented in the MOLPRO package and to describe nuclear quantum effects at Hartree-Fock level of theory with the APMO code. Different model systems illustrate the implementation: $^4He_2$ dimer as a protype of a weakly bound van der Waals system; isotopomers of $[He–H–He]^+$ molecule as an example of a hydrogen bonded system; and molecular hydrogen to compare with very accurate non-Born-Oppenheimer calculations. The possible improvements and future developments are outlined.

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