Theoretical investigation of hydrogen isotope effects in water dimers

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We have studied the effects of gradual hydrogen isotope substitution on the geometries, energetics and properties of water dimers.
We have carried out all calculations with the APMO code, which implements the nuclear orbital and molecular orbital approach at the HF and MP2 levels of theory for electrons and hydrogen nuclei.
Our results are in agreement with experimental data and are key for the understanding of hydrogen isotope effects on larger water aggregates.