From H_5 to larger protonated hydrogen clusters PES and Dynamics

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ABSTRACT

Results of recent studies on the H_{2n+1}^+ clusters will be presented. Nowadays for the first members of this series high accurate ab initio electronic structure calculations can be carried out. However, a reliable global representation of even the H_5^+ PES is still an open and challenging problem[**?**]. Thus, here an alternative approach following the idea of ab initio molecular dynamics simulations, that combines nuclear dynamics methods with first principles electronic structure calculations within the DFT framework is adopted. Such DFT approach using the B3(H) hybrid functional specially designed for hydrogen-only systems, allows to carry out reliable dynamics calculations, by computing the potential value at a given configuration, on the fly, with both reasonable accuracy and at low computational cost without any posterior parametrization procedure of the surface[**?**]. It was found taht the DFT / B3(H) approach provides a reliable global description of the potential surface of the H_5^+ cluter. Based on the B3(H) surface both classical and path integral Monte Carlo (CMC, PIMC) calculations at low temperature are carried out to investigate quantum efects on the internal proton transfer and thermal structural fluctuations on the vibrational zero-point structure of H_5^+ cluster[**?**]. Such findings are of particular interest for studying larger species of the H_n^+, as well as gas-phase solvation effects, cluster fragmentation, and collision processes in astrophysical applications[**?**],[**?**],[**?**],[**?**],[**?**],[**?**]

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