Ionized helium clusters: quantum effects

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The main objective of the present study is a detailed theoretical description of structural properties, stability, and energetics of ionized helium clusters. Our objects are interesting due to experiments performed in helium nanodroplets at very low temperatures and weak perturbations, taking benefits of helium superfluidity. For theoreticians, the field of ionized helium clusters is the great challenge, too. On the one hand, there is a failure of the semiempirical *diatomics-in-molecules* interaction model (successful for heavier rare gas clusters) due to an insufficient inclusion of three-body forces; on the other hand, for these quantum systems of light nuclei it is not possible to use only stationary points on potential energy surfaces for exact calculations of ground state properties of these species. In the light of an exact analysis [1] performed for similar systems, Ne^+He_n, we can expect a strong quantum behavior for He_n^+ as well as experimental magic numbers not fully compatible with simple considerations based on the analysis of stationary points only. In addition, strong anharmonic effects in He_n^+ don't allow us to use a simple harmonic approximation and, therefore, we used stochastic quantum diffusion Monte Carlo method to describe the clusters. The results obtained via simulations have been compared with experiments (see e.g. [1]). The helium ionized trimer is the ionic core for most of clusters sizes, and the analysis of He_3^+ has thus been performed with a special care. We also computed vibrational spectrum of the He_3^+ using the hyperspherical method for several different potential energy surfaces. The effect of the geometrical phase appears as a non-negligible factor for higher, delocalized excited vibration states [2].

[1] C.A. Brindle, M.R. Prado, K.C. Janda, N. Halberstadt, and M. Lewerenz, J. Chem. Phys. 123, 064312 (2005)
[2] F. Karlický, B. Lepetit, R. Kalus, I. Paidarová, and F.X. Gadéa, J. Chem. Phys. 128, 124303 (2008)