Path Integral Monte Carlo calculations on atomic clusters


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Classical and quantum Path Integral Monte Carlo (PIMC) calculations have been performed to study two different kinds of atomic clusters. In the first part, heavy-atom microcluster Ar$_3$ in the temperature range from 1 K to 40 K was studied$^1$. PIMC results using different confinement radii were compared with other theoretical approaches, such as Distributed Gaussian Function (DGF) method$^2$ and simple analytical models involving either the discrete (Model I) or both the discrete and continuum spectrum (Model II) (see top figure). The main conclusion is that the influence of the continuum is determinant in the dynamics of small clusters beyond a critical temperature.

In the second part we focus our research on ionic hydrogen clusters, which are relevant in astrophysics due to their presence in interstellar clouds and atmospheres of jovian planets$^3$. Structural and energetic properties of H$_5^+$ and its fragments H$_3^+$ and H$_2$ were calculated at low temperature$^4$, via "on fly" ab initio path integral Monte Carlo calculations, employing a DFT functional specially designed for hydrogen-only systems. This approach allows us to obtain a low computational cost surface that describes all the particular features of H$_5^+$$^5$. In this way we achieve fully converged ab initio PIMC results for the thermostatics of the cluster. Of particular relevance are the vibrational zero-point energies (ZPE) and states and the dissociation energy D$_0$ (see bottom figure). Results will be discussed and compared with other calculations and experimental measurements$^6$.

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