

Quantum Chemistry-like and Path Integral Calculations on Doped Helium Clusters

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Synopsis For molecular species immersed in or attached to helium clusters, quantum chemistry-like and Path Integral calculations are presented and discussed.

We review some theoretical studies carried out in our group involving molecular species immersed in (or attached to) He clusters at very low temperatures. Using a quantum chemistry-like methodology, superfluidity of boson ^4He (in contrast with fermion ^3He) clusters is demonstrated for dopants residing inside the droplet by spectroscopic IR or Raman simulations depending on their polar or non-polar nature [1, 2, 3, 4]. Also, Path Integral Monte Carlo (PIMC) calculations are used to determine the energy and structure for different atomic, molecular and ionic species sometimes placed at the surface of boson He droplets [5, 6, 7, 8]. Fig 1 displays initial configurations obtained through an evolutive algorithm for further PIMC simulations of small $^4\text{He}_N$ clusters doped with an $^4\text{He}^{*-}$ anion [7, 8].

In turn, Fig 2 displays the formation of a rubidium dimer on a $^4\text{He}_{70}$ cluster obtained using a coloured thermostat in a Path Integral Molecular Dynamics (PIMD) simulation with the i-PI package [9]. The approaching of rubidium atoms evolves inside the helium aggregate and eventually the Rb_2 emerges towards the surface of the cluster.

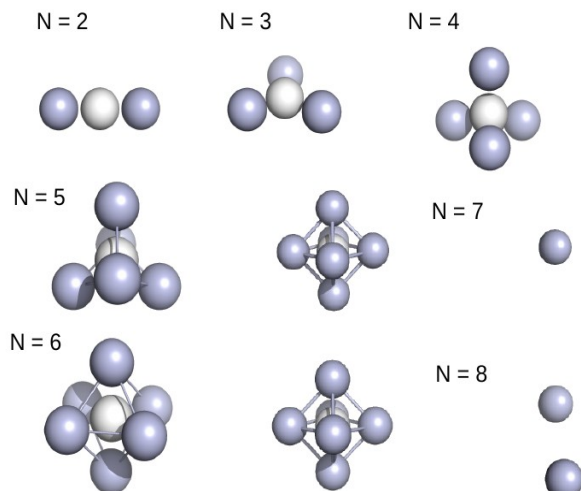


Figure 1. Initial configurations of $^4\text{He}_N$ - $^4\text{He}^{*-}$ anionic clusters.

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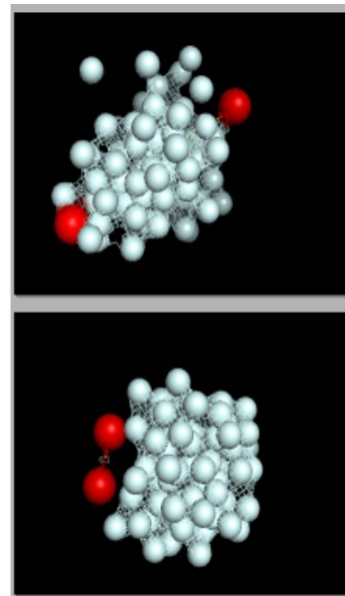


Figure 2. $^{87}\text{Rb}_2(^3\Sigma_u^+)$ - $^4\text{He}_{70}$ complex: Initial configuration (upper panel) and final one (lower panel) after a PIMD simulation at $T=2$ K.

References

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