Variational and Path Integral Monte Carlo calculations on Helium Clusters Doped with Metastable Anions He^{*-} and He_2^{*-}

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Variational and Path Integral Monte Carlo calculations on Helium Clusters Doped with Metastable Anions He^{*-} and He_2^{*-}

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Synopsis Variational calculations (T=0 K) on small He_N...He^{*-} and He_N...He_2^{*-} metastable clusters (N≤4), as well as Path Integral Monte Carlo (PIMC) simulations (T=0.4 K) on larger species are presented and discussed.

The calculations[1] have been carried out assuming additive pairwise-like potential surfaces. The underlying He(^{1}S)-He^{*-}(^{4}P) potential curve and the He(^{1}S)-He_2^{*-}($^4\Pi_g$) anisotropic interaction have been recently estimated through accurate CCSD(T) calculations[2]. The He-He interaction is described by a semi-empirical potential[3].

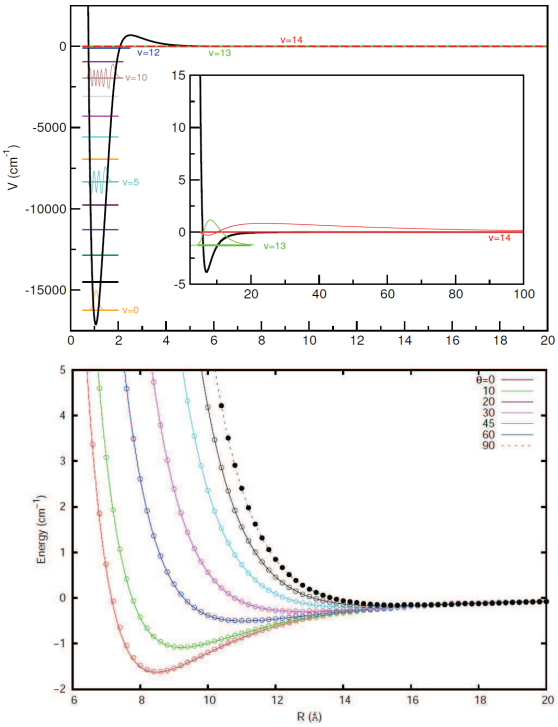

Figure 1. He-He^{*-} potential curve supporting 15 bound states, the last two ones being depicted in the inset (upper panel), and He-He_2^{*-} anisotropic interaction (lower panel).

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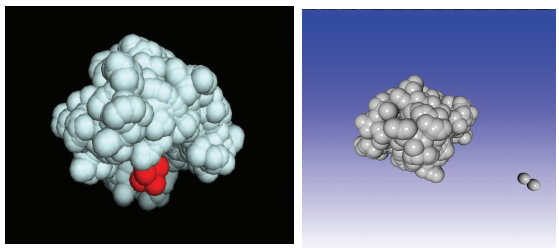

Figure 2. Left panel: snapshot from the PIMC simulation for the He_{32}-He^{*-} cluster at T = 0.4 K showing a bi-pyramid anionic structure surrounded by the rest of He atoms. Right panel: the simulation for the He_8-He_2^{*-} cluster shows instead the impurity far away the helium cluster.

For the atomic anion case, the interaction with helium presents a deep well near 1 Å followed by a small barrier and then a shallow minimum, see upper panel at **Figure 1**. Accordingly, as He atoms are added, a marked preference to form a bi-pyramid charged core He_7^-, with the rest of He atoms surrounding it, is obtained through PIMC simulations, see **Figure 2** (left panel).

In turn, the molecular anion He_2^{*-}, considered as a rigid rotor, tends to point towards a set of packed helium atoms which are placed at long distance from the anion, see **Figure 2** (right panel).

References

[1] R. Rodríguez-Cantano *et al* 2015 *J. Chem. Phys* **142**, 104303

[2] S. E. Huber and A. Mauracher 2014 *Mol. Phys.* **112**, 794

[3] R. A. Aziz and M. J. Slaman 1991 *J. Chem. Phys.* **94**, 8047