Variational and Path Integral Monte Carlo calculations on Helium Clusters Doped with Metastable Anions He*− and He2*−


*IFF-CSIC, Serrano 123, 28006 Madrid, SPAIN
†Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Technikerstr. 25, A-6020 Innsbruck, AUSTRIA

Synopsis Variational calculations (T=0 K) on small HeN...He*− and HeN...He2*− 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(1S)-He*−(4P) potential curve and the He(1S)-He2*−(4Πg) 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 2. Left panel: snapshot from the PIMC simulation for the He8-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 He8-He2*− 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 He7−, with the rest of He atoms surrounding it, is obtained through PIMC simulations, see Figure 2 (left panel).

In turn, the molecular anion He2*−, 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
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Figure 1. He-He*− potential curve supporting 15 bound states, the last two ones being depicted in the inset (upper panel), and He-He2*− anisotropic interaction (lower panel).

1E-mail: p.villarreal@csic.es