Quantum Monte Carlo study of Rb^*, Rb_2 and other alkali in helium clusters

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Spectroscopy of doped helium nanodroplets has become, in recent years, a popular tool for the study of both finite size samples of the helium quantum fluid and molecules isolated in this sub Kelvin environment. While many dopants migrate to the center of the droplet, alkali (Ak) atoms in their ground electronic state, because of their so weak interaction with He, remain at the surface, the latter being in this way slightly distorted exhibiting a dimple. However, when in their first excited states, Ak atoms are forming exciplexes. These are anisotropic with the central atom surrounded by a ring of He atoms located in the nodal plane of the valence electron p_z orbital. Structural properties, obtained by DMC and PIMC, are presented here for some Ak^* - He_n exciplexes.
Ak_2 dimers in helium environment have also gained interest in this last decade, in connexion with the generation of ultracold molecules. When attached to helium droplets, Ak atoms can float on the surface and form molecules in cold collisions. DMC and PIMC methods are used to compute energetics and structural informations for Rb_2 in helium. In particular, the orientation of the dimer relative to the droplet surface is examined.

1. Leino, M., Viel A., Zillich R., (2008). "Electronically excited rubidium atom in a helium cluster or film". The Journal of Chemical Physics 129, 184308.

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