ALKALI DIMERS: A CASE OF NOT SOLVATED IMPURITIES IN HELIUM CLUSTERS

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Helium clusters is a topic widely studied up to date and a huge wealth of theoretical and experimental works is in the literature. The usual scenario is an impurity, or ensemble of impurities, inside the helium environment. The rare gas atoms form an inert substrate in which the dopant can be analyzed in specially favourable conditions (sometimes the only manner to do it).

Alkali atoms show a very special feature compared with the others: they are not solvated for the droplet and remain in the surface. The question about whether or not the alkali dimers adopted also this arrangement came up immediately and the articles answered in an affirmative way, for instance, in the case of Li_2 [1]. Molecules like K_2, Rb_2, and Cs_2 have been experimentally researched by the groups of Ernst and Stienkemeier. However, very little theoretical work can be found.

So, we decided to face the problem applying a Diffusion Monte Carlo methodology to small complexes formed by an alkali dimer and some Helium atoms, in particular, $Cs_2(^3\Sigma_u)$-$(^4He)_N$ and $Rb_2(^3\Sigma_u)$-$(^4He)_N$, $2 \leq N \leq 20$. Our results are in agreement with the previous one, and we find a picture in which the whole cluster is more stable with respect to the pure rare gas partner, but there is a segregation of the diatom and the Helium atoms, being apart one from the others. We think that this is so because of the more strong He-He potential in comparison with the dimer-He one.

There is still a big amount of pending research in the alkaline group, for instance, the charged dimers, and future work is oriented in this direction. For a better comprehension of the problem multi-orbital-Hartree [2] and Path Integral Monte Carlo [3] approaches have been applied. The results will be relevant not only in the field of Helium clusters, but also in related areas like cold and ultracold collisions, hence the necessity to keep working on it.

References

[1] S. Bovino, E. Coccia, E. Bodo, D. López-Durán, and F. A. Gianturco, *J. Chem. Phys.* **130**, 224903 (2009).

[2] M. P. de Lara-Castells, D. López-Durán, G. Delgado-Barrio, P. Villarreal, C. Di Paola, F. A. Gianturco, and J. Jellinek, *Phys. Rev. A* **71**, 033203 (2005).

[3] R. P. de Tudela, D. López-Durán, T. González-Lezana, G. Delgado-Barrio, P. Villarreal, F. A. Gianturco, and E. Yurtsever, submitted to *J. Phys. Chem. A*.