Path integral Monte Carlo calculations of Ca impurity in helium droplets

R. Rodríguez-Cantano¹, D. López-Durán¹, T. González-Lezana¹, F. A. Gianturco², G. Delgado-Barrio¹ and P. Villarreal¹

¹ Institute of Fundamental Physics, IFF-CSIC, Madrid, Spain
² Department of Chemistry and CNISM, University of Rome La Sapienza, Italy

E-mail: rrcantano@iff.csic.es

Helium clusters have been successfully employed as an ideal environment to spectroscopically investigate an ample list of impurities. For the case of atoms, the question of establishing solvation or surface location for the impurity in the helium droplet is an issue of great importance to further understand its behavior and the spectroscopic observations.

A crucial aspect which needs to be taken into consideration for these systems is the dopant-solvent interaction. In particular, in the case of the Ca atoms, the He-Ca potential energy curve (PEC) has been studied and reported through various publications in recent years: The modeling of it via simple empirical formulae was put forward by Kleinekathöfer in the year 2000 [1], where he found a well depth of 10.3 cm⁻¹ at a distance of 5.1 Å. Earlier calculations of Stienkemeier et al. [2] had provided a well depth of 11.6 cm⁻¹ at a distance of 5.45 Å, similarly to recent Tang’s predictions [3] of 12.42 cm⁻¹ and 4.9 Å, respectively. On the other hand, *ab initio* quantum chemical calculations indicate a very different scenario: the work of Lovallo and Klobukowski [4] found an equilibrium distance of 6.02 Å and a well depth of 3.32 cm⁻¹ in line with calculations carried out by Czuchaj et al. [5], K. Partridge et al. [6], and the very accurate quantum chemical study of Hinde [7].

In this work we present path integral Monte Carlo (PIMC) [8] calculations of ⁴Heₙ nanodroplets doped with a single calcium atom at low-temperature range. Simulations have been carried out using different He-Ca interactions, revealing substantial discrepancies regarding the precise location of the Ca impurity with respect to the helium droplet and the binding energy of the system.