Structure and Spectroscopy of Helium Nanodroplets Doped with Molecular Impurities at Low Temperatures.

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Abstract

We review in this talk some theoretical studies carried out in our group involving molecular species immersed in (or attached to) He clusters at very low temperatures. Using a quantum chemistry-like methodology, superfluidity of boson ^{4}He (in contrast with fermion ^{3}He) clusters is demonstrated for dopants residing inside the droplet by spectroscopic IR or Raman simulations depending on their polar or non-polar nature[1-4]. In addition, Path Integral Monte Carlo calculations are used to determine the energy and structure for different atomic, molecular and ionic species frequently placed at the surface of boson He droplets[5-8].

References

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Figures

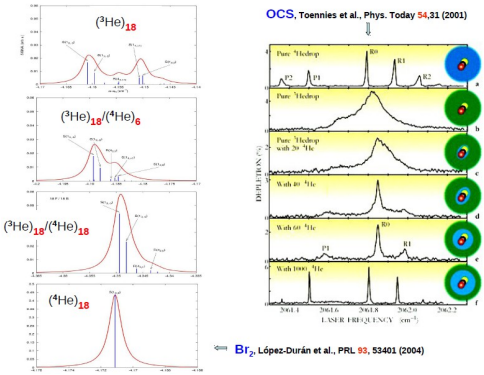

Fig 1: Evolution of S branches in the Raman spectra of Br_2 embedded in different mixtures of ^{3}He/^{4}He clusters at T=0.5 K[1].

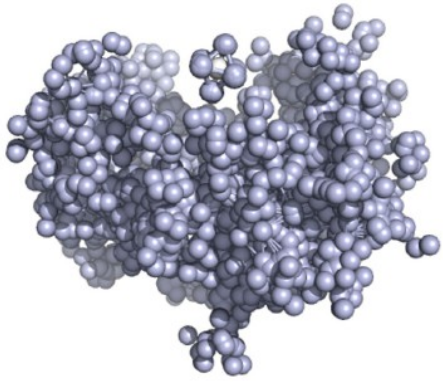

Fig 2: Snapshot from the PIMC simulation for $He_{32}-He^{*-}$ at T = 0.4K. A bipyramid structure can be seen in a dimple at the top[8].