

Title: Chemistry involving superfluid helium droplets as a solvent.

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In the early 1960s, a way to synthesize superfluid helium nanodroplets was found, and in 1990 the capture of atoms and molecules by helium nanodroplets was reported for the first time. In this work, an introduction into the field of the doped superfluid helium nanodroplets is given with emphasis on the chemical perspective. The fundamental background of all the aspects discussed is explained, always keeping in mind that the aim of this work is to provide a first contact to this interesting but intricate topic. Here, we present a brief introduction on the superfluid helium nanodroplets, followed by a review on the most important experimental and theoretical methods available to investigate these systems.

In the experimental section, the most relevant techniques used to extract information from helium nanodroplets are shown. Spectroscopic techniques allow to elucidate the structures of the impurities in the nanodroplets. Pump-probe laser techniques provide a way to determine dynamic information that deepens our insight on very low-temperature chemical reactions among other processes. The special properties of helium nanodroplets allow us to find new products, such as metastable pre-reaction complexes, cold-channel products and even complex nanostructures unobtainable otherwise.

In the theoretical section, the different methods available to simulate chemical phenomena occurring within helium nanodroplets are reviewed. Fully quantum mechanical structure calculations are beyond the computational possibilities for nanodroplets of hundreds or thousands of He atoms and the description of the systems must be carried out employing a hybrid approach. In structure investigations helium nanodroplets are described using density functional theory, while the impurities (atoms or molecules) can be described employing *ab initio* or classical approaches depending on the system studied. Dynamic studies have recently been developed using similar hybrid methods. Generally, the impurities are described using quantum or classical mechanics and the superfluid helium is described using time dependent density functional theory. Several methods that use different approaches can be applied to investigate processes involving doped helium nanodroplets.

Keywords: Superfluid helium nanodroplets, quantum solvent, low temperature, chemical processes.