Clustering dynamics in superfluid helium nanodroplets: A theoretical study

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In this work we study the collision of heliophilic atoms with a superfluid helium droplet, followed by their solvation and clustering. ^{4}He nanodroplets are intriguing, quantum fluid objects of finite size (typically several thousands of ^{4}He atoms) [1]. They exhibit very "exotic" properties, including superfluidity, very low temperature (0.38 K), high energy dissipation rate, quantum vortices,... They constitute an interesting medium to study molecules at very low temperatures, even lower than the interstellar medium. Because of their very high energy dissipation rate, they can trap collisional complexes in local, metastable configurations which may be of interest for comparison with, eg, photo-association complexes when the ground, thermodynamic configuration is not attained.

We use time-dependent Helium density functional theory (^{4}He-TDDFT), which has proven to be the best compromise between accuracy and feasibility to study the stability and real time dynamics of doped helium droplets with a size comparable to experiments.[2]

We also investigate the effect of the presence of a quantum vortex on the pickup and clustering process, in relation with the pioneering experiment by Vilesov's group which used atom doping to visualize quantum vortices.

Our simulations[3, 4] reveal rather surprising final cluster configurations, very different from the gas phase ones. This is due to the fast cooling property associated to superfluidity, which quenches metastable configurations, and to the high density shell building around each dopant atom which can prevent dopant-dopant bond formation. They also reproduce the attractivity of dopant atoms to the vortex lines, with a cluster building along them but in a final configuration very different from the gas phase one. We also compare the results of ^{4}He-(TD)DFT simulations in vortex free nanodroplets with particle-based methods which have been used for these systems.[5]

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