

# Structure, dynamics, and superfluidity of small doped He clusters

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Helium clusters and nanodroplets constitute an ideal matrix to study the properties of molecular species in an ultracold environment. At the same time, the spectroscopy of molecular impurities solvated in Helium provides a unique opportunity to probe the behavior of quantum fluids in confined geometries. Progress in this field is being burst by recent advances in Helium droplet isolation spectroscopy, on one hand, and in computer simulation on the other. Thanks to these advances, the relation of the structure of the solvent with the dynamics of the solvated molecule, and of both with the appearance of fingerprints of “superfluidity” in these confined systems are now being unveiled.

In the first part of my talk, I will briefly review the foundations of *Reptation Quantum Monte Carlo*, a simulation technique from which static ground-state properties (such as binding energies, atomic density distributions, and correlation functions) as well as dynamic correlations (which give information on excitation energies and absorption oscillator strengths) can be estimated without any systematic errors. I will then proceed illustrating the results of computer simulations recently carried out for  $\text{OCS@He}_n$  and  $\text{CO@He}_n$  in the size range  $n=3-20$ , for which fresh experimental data exist. In the first case, the rotational spectrum of the complex consists of just one line per angular momentum, as for the isolated molecule. The effective molecular moment of inertia, calculated as a function of the cluster size, agrees well with experimental data when these are available, and provide predictions when they are not. In all cases, a comparison between the calculated spectrum and the structural properties of the complex in its ground state provides a deep insight onto the onset of “superfluidity” in this system. The rotational spectrum of  $\text{CO@He}_n$ , instead, is not directly known experimentally, and it could only be deduced from the rotational structure of the vibrational lines. The available experimental information, however, is not sufficient to disentangle the rotational features in the vibrational spectrum, and simulations help explain the number, position, and intensity of the observed lines in terms of the size and shape of the complex.