Clustering dynamics in superfluid helium nanodroplets: A theoretical study

Ernesto García Alfonso,[1] *Manuel Barranco,*[1,2,3] *David A. Bonhommeau,*[4]
Florent Calvo,[5] *Martí Pi,*[2,3] *and* Nadine Halberstadt[1]

[1]LCAR, CNRS and Université Toulouse 3, F-31062 Toulouse, France
[2]Departament FQA, Facultat de Física, Universitat de Barcelona, Barcelona, Spain
[3]Institute of Nanoscience and Nanotechnology (IN^{2}UB), Universitat de Barcelona, Barcelona, Spain
[4]Université de Reims Champagne Ardenne, CNRS, GSMA UMR 7331, 51100 Reims, France
[5]Université Grenoble Alpes and CNRS, LIPHY, F-38000 Grenoble, France
Nadine.Halberstadt@irsamc.ups-tlse.fr

We report theoretical investigations on the dynamics of doped ^{4}He nanodroplets (HeND) in real time. HeND are intriguing, quantum fluid objects of finite size (typically several thousands of ^{4}He atoms) [1]. Their properties include superfluidity, very low temperature (0.38 K), high energy dissipation rate, quantum vortices,...

Helium density functional theory (^{4}He-DFT) and its time-dependent version (^{4}He-TDDFT) have 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] They constitute a phenomenological approach based on a fluid description of the helium droplet at 0 K. The parameters of the functional have been adjusted to reproduce various properties of the bulk superfluid liquid.[2]

In this work we study the collision of heliophilic atoms with a droplet, followed by their solvation and clustering.[3, 4, 5] In particular, we investigate the effect of the presence of a quantum vortex in the droplet, in relation with the pioneering experiment by Vilesov's group which used Ag, Ar or Xe atom doping to visualize quantum vortices [6]. Our simulations indeed reproduce the attractivity of dopant atoms to the vortex lines, with a rather surprising final cluster configuration, very different from the gas phase one.[4, 5]

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.[7] The ring-polymer molecular dynamics (RPMD) method[8] uses a path-integral description of nuclear motion, and incorporates zero-point delocalization while ignoring bosonic exchange effects. The zero-point averaged dynamics (ZPAD) approach[9] is a mixed quantum-classical method in which quantum delocalization is described by attaching a frozen wave function to each He atom, equivalent to classical dynamics with effective interaction potentials.

Index Terms: superfluid helium nanodroplets, helium density functional theory, collision and clustering

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