

Solvation of alkali ions in helium droplets: an atomistic perspective on the mechanisms and associated time scales

F. Calvo

Laboratoire Interdisciplinaire de Physique (LiPhy), CNRS & Université Grenoble Alpes, France

Abstract: The post-ionization solvation of heliophobic alkali atoms in contact with helium droplets was recently investigated experimentally [1] by pump-probe spectroscopy, using an auxiliary, heliophilic xenon ion as a repelling center. In the present contribution, the experimental system has been theoretically modeled through the various ionization and solvation steps, up to the ejection of the alkali possibly solvated by a number of helium atoms, using ring-polymer molecular dynamics simulations employing accurate interaction potentials for the sodium and potassium cases. With the aim to provide a statistical picture of the ejection of the microsolvated alkali ion, we notably examine the time-dependent mechanisms of how the solvent coats the ion at the earliest stages following ionization, and find that the solvation is concomitant with a significant diving of the ion inside the droplet. Compared to sodium, the greater heliophilic character of potassium leads to smaller solvation shells upon ejection.

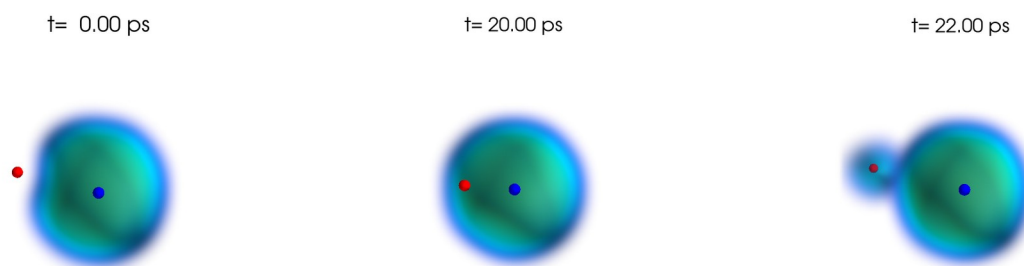


Fig 1. Ionization of a sodium atom (in red) in contact with a 1000-atom helium nanodroplet, followed after 20 ps by the ionization of the xenon atom (in blue), as simulated using ring-polymer molecular dynamics simulations

References:

1. S. H. Albrechtsen *et al.*, *Nature* (2023), **623**, 319.