Concurrent processes in the time-resolved solvation of alkali ions in helium nanodroplets

Florent Calvo[a]

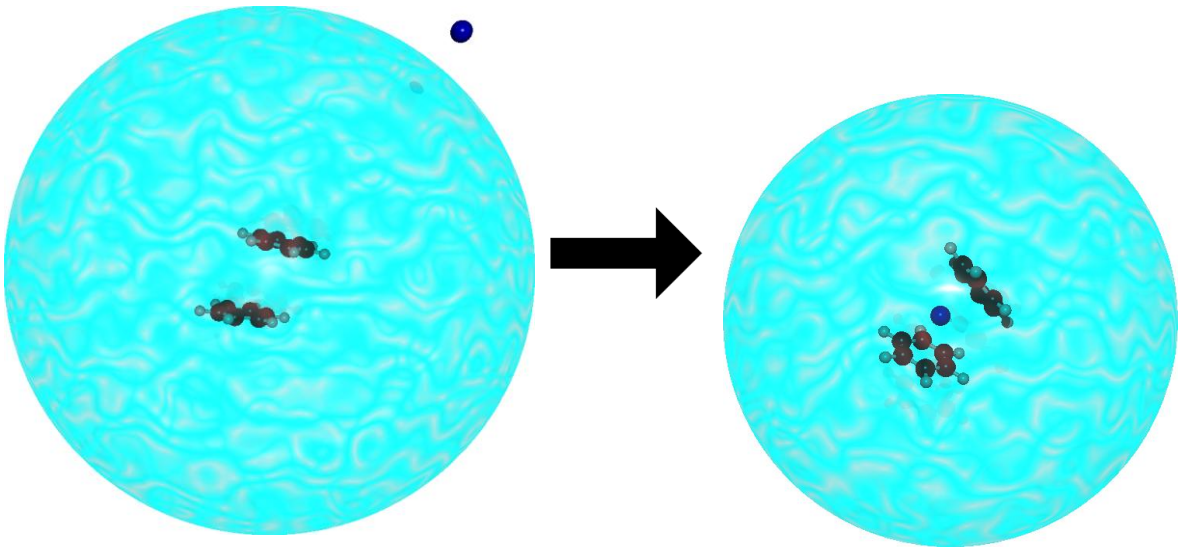
[a]*Université Grenoble Alpes, CNRS, LiPhy, F38000 Grenoble, France*

florent.calvo@univ-grenoble-alpes.fr

Recent pump-probe experiments [Albrechtsen *et al.*, Nature **623**, 319 (2023)] have explored the gradual solvation of sodium cations in contact with helium nanodroplets, using a fully solvated xenon atom as a probe exerting a repulsive interaction after its own ionization. In this contribution, we computationally examine by means of atomistic ring-polymer molecular dynamics the mechanisms of successive ionizations, shell formation, and Coulomb ejection that all take place within tens of picoseconds, and show that their interplay subtly depends on the time delay between the two ionizations but also on the droplet size. The possibility of forming solvated Na^+Xe non-covalent complexes under a few tens of picoseconds in such experiments is ruled out based on fragment distributions.

Besides accounting for the main phenomenology of the sodium-xenon experiment, we extend the investigation to the case of potassium, still with the xenon dopant, and predict significantly smaller, partially solvated K^+ cations, owing to the even weaker interaction in the neutral state.

Finally, our first results involving molecular dopants (benzene, cyclohexane, and their dimers) will be presented.



References

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