# Tracking microhydration of salt molecules by Penning ionization electron spectroscopy in helium nanodroplets

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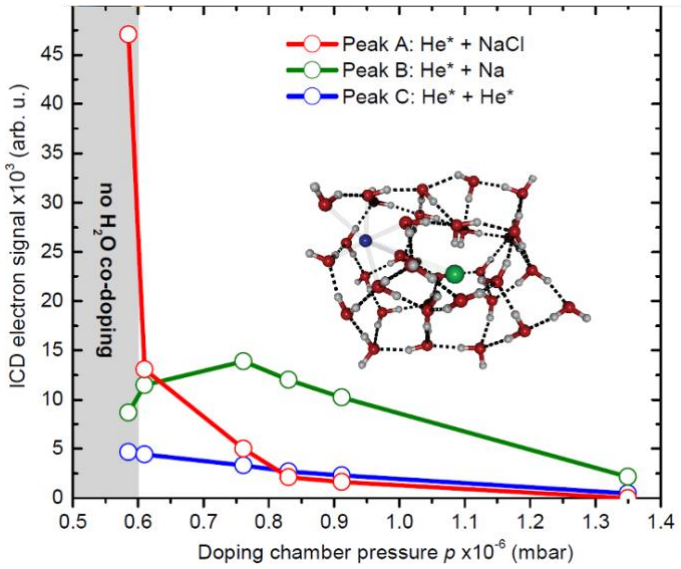
The microhydration of salt molecules (NaCl, NaBr, KBr) is investigated by Penning ionization electron spectroscopy (PIES) in helium nanodroplets [a]. Although model calculations predict that NaCl molecules are fully submerged inside the droplets, PIES of NaCl are highly resolved, similar to surface-bound alkali-metal atoms. PIES of salt molecules reveal efficient simultaneous ionization and excitation into high-lying charge-transfer states; benchmark measurements on alkaline-earth metals (Mg) show that only simultaneous ionization and excitation leads to the ejection of atomic ions from the helium droplets, whereas ground-state $Mg^+$ ions remain bound to the droplets.

Adding to the NaCl-doped helium droplets a controlled number of $n$ = 1-10 water molecules leads to efficient quenching of NaCl Penning ionization and to its full suppression for $n$ > 30, see the red line in the figure below. Accompanying density-functional theory (DFT) and force field (FF) calculations reveal a transition from contact ion pair structures to solvent-separated ion pairs at $n$ = 12-15. However, it takes $n \approx 17$ water molecules to form a complete solvation shell around the $Cl^-$ anion and as many as $n \approx 34$ to fully hydrate the $Na^+$ cation, thus the entire NaCl molecule, which rationalizes the experimental findings. In addition to presenting these recent results, I will report on the progress of research activities in WG4.




*Electron signals measured for Penning ionization of NaCl, Na and excited He* embedded in helium nanodroplets as a function of the vapor pressure of water co-doped into the droplets. The inset shows the structure of NaCl solvated by a cluster of 34 water molecules obtained from force field (FF) exploration.*

References:

[a] Ben Ltaief, L., Sishodia, K., Richter, R., Pi, M., Barranco, M., Eloranta, J., Krishnan, S.R., Calvo, F., Mudrich, M., Tracking Microhydration of the NaCl Rocksalt Molecule in Helium Nanodroplets by Penning Ionization Electron Spectroscopy, submitted to Small Structures, 2026; https://doi.org/10.XXX arXiv:2510.22000.