Computer simulations of helium-solvated ions: solid-like versus liquid-like defect structures STEFANO PAOLINI, FRANCESCO AN- CILOTTO, FLAVIO TOIGO, INFM-DEMOCRITOS National Simulation Center (Trieste, Italy) and Physics Department “G. Galilei”, University of Padova (Italy) — The local order around several alkali (Li$^+$ and Na$^+$) and alkali-earth (Be$^+$, Mg$^+$ and Ca$^+$) ions in $^4$He clusters has been studied using ground-state path integral Monte Carlo simulations. We apply a criterion based on multipole dynamical correlations to discriminate between solid-like versus liquid-like behavior of the He solvent surrounding the impurity-ion. In agreement with existing experimental measurements in bulk helium, our findings suggest that Be$^+$ produces a solid-(“snowball”)-like structure, similarly to alkali ions and in contrast to heavier alkali-earth ones, for which a liquid-like environment is predicted.

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