Attachment of hydrogen molecules to atomic ions: role of the hydrogen rotational states

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Interactions between molecular hydrogen and ions are of interest in cluster science, astrochemistry and hydrogen storage. In dynamical simulations, H_2 molecules are usually modelled as point particles (pseudoatoms), an approximation that can fail for anisotropic interactions. Here we apply an adiabatic separation of the H_2 rotational motion to build effective pseudoatom-ion potentials and in turn study the properties of $(H_2)_nNa^+/Cl^-$ clusters. The potentials are based on high-level *ab initio* calculations and improved Lennard-Jones parametrizations, the subsequent dynamics being performed by Difussion Monte Carlo calculations. By comparisons with simulations explicitly describing the molecular rotations, it is concluded that the present adiabatic model works very well. Interestingly, we find differences in the cluster stabilities and coordination shells depending on the spin isomer considered (para- or ortho-H_2), specially for the anionic clusters.