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A theoretical study on hydration of alanine zwitterions

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Abstract

Structures and energetic of hydrogen bond (H-bond) networks of water at the charged functional groups of two forms of alanine zwitterions were studied using various theoretical methods. The present investigation started with a construction of intermolecular potentials between the zwitterions and water followed by Molecular Dynamics (MD) simulations of aqueous solutions. The three-dimensional structures and the average potential energy landscapes of the H-bond networks of water were analyzed and visualized using various probability distribution (PD) maps. Although the conformation with planar skeleton possesses larger overall stabilization by hydration, the conformation with the COO^- plane being 90° with respect to the $NC^{\alpha}C$ backbone seems to be more accessible by water. The MD analyses revealed that, although the shapes of the average potential energy landscapes at the H-bond networks are highly irregular, they can help characterize the dynamic behavior of water molecules especially at the functional groups the solutes.
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Keywords: Alanine zwitterion; Hydrogen bond; Aqueous solution; Molecular dynamics simulations

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