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The effect of intermolecular hydrogen bonding on the polyaniline water complex

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ABSTRACT

The polymer water hydrogen-bonded complex was studied by computer modelling and simulation using *ab initio* calculations. The density functional theory (DFT) method was used to calculate the structure characters, natural bond orbital (NBO) charge distribution, infrared spectra as well as the frontier molecular orbital. Results showed that the H–O···H–N and C–N···H–O type intermolecular hydrogen band structures were formed. The chemical bonds involved in the intermolecular H-bond were all influenced by the hydrogen bonding interaction, especially for the bonds which provided hydrogen atom for the H-bond were elongated uniformly. During the hydrogen bond formation, the polymer chains in the complexes were all charged compared with the neutral PANI monomer, and the charge of the chains was redistributed in the complexes, which can be an important factor contributing to the increase in electrical conductivity. The N1–H vibration was strongly influenced by the hydrogen bond, and the locations and the intensities of N1–H absorption bands were all changed in the complexes. In addition, we also discussed the frontier molecular orbitals and the electron density transition. In the orbital transition of HOMO to LUMO, the electron density transferred from benzenoid ring to quinoid ring.