**Abstract**

Density functional theory (DFT) calculations followed by molecular dynamics study has been performed to analyze the structure and stability of β-dipeptide structures in aqueous medium. From DFT study, three local minima with folded conformations and one local minimum with unfolded conformation have been identified. In gas phase, the most stable β-dipeptide has a folded conformation with a weak hydrogen bonding. The interaction of water molecules, approximated from the first solvation shell, also confirms the folded conformation to be the most stable structure. The DFT optimized β-dipeptide conformers have been simulated in explicit water to evaluate the tendency of folded and unfolded state formation. Simulations confirmed the transition of the structure from folded to unfolded and vice versa and further indicated the former to happen rapidly within a few pico second time scale.