ABSTRACT

Water is one of the most important solvents due to its large compound on earth. Water is essential for many chemical reactions, the fluids of all known living organisms, and the main component of biological systems. However, the structure of the molecular water ensemble in the vicinity of the polymers is under discussion. During the past few decades, many experimental and theoretical studies have investigated the hydrated polymer to clarify its structure, especially polymers' bio/blood compatibility. The interactions between water and polymers are dependent on structure, polarity, hydrophilicity or hydrophobicity, and functional groups. In this study, we use the molecular dynamics method to analyze the structure of water in the vicinity of bioactive polymers onto gold surface at various temperatures. The different amounts of TIP3P/B water and external electric field are also considered. Water distributions around functional groups, hydrogen bond network, and tetrahedral order are analyzed to classify various types of water around the polymer. We discovered a tight association between water's tetrahedral arrangement and its XES experiment. We found that four water zones are separating from one another in the range of 1 to 6 Å around polymers. As a result of interactions between water molecules and functional groups like hydroxyl, ether, and ester, intermediate and non-freezing water is generated.