

Aggregation of Polysorbate 80 in room temperature ionic liquids investigated by molecular dynamics simulations

ABSTRACT

The ability of room temperature ionic liquids (RTILs) to act as media for self-aggregation of amphiphilic molecules have been widely reported. However, insights on how the self-aggregation of amphiphiles occur in RTILs at the atomic level is very important to further utilize its potential. Here, the ability of a non-ionic surfactant to self-aggregate in RTILs was modelled and evaluated using computational approach. Molecular dynamics (MD) simulations were carried out to model the self-aggregation process of Polysorbate 80 (T80) in water and in 1-butyl-3-methylimidazolium hexafluorophosphate, [BMIM][PF₆] and 1-butyl-3-methylimidazolium tetrafluoroborate, [BMIM][BF₄]. The aggregation behaviour of T80 in water and both RTILs were observed during 50 ns of MD simulations. In comparison to water, the self-aggregation of T80 was found significantly slower in both RTILs. Simulation results revealed weak solvophobicity of RTILs in comparison with the hydrophobic effect in water. The effect of different anions was unclear, possibly due to the equal ability of both RTILs to facilitate self-aggregation when compared with water. A spherical model of T80 aggregate was built and then simulated in water and in both RTILs. Results indicated that the aggregate had better structural stability in RTILs than in water.

Keyword: Self-aggregation; Polysorbate 80; Ionic liquids; Molecular dynamics