Fundamental Mechanism of Chemical Depolymerization of Thermoplastics in Ionic Liquids: Molecular Dynamics Study

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The mechanism of chemical depolymerization of waste plastics using ionic liquids was investigated by the molecular dynamics (MD) study. Two constituent polymers in thermoplastics are under our investigation. One is Nylon-6 using [PP13][TFSI]. The other is PET using [Bmim][Cl]. In this study, the bond extension beyond equilibrium length is treated as the onset of the bond breakage. Thus, all bonding energies in the repeat unit of polymer were calculated by density functional theory and the bond length distributions were analyzed in the presence of ionic liquid to determine the bond breakage criteria. In lieu of the MD information obtained, exact identities and numbers of broken bonds were captured in the atomistic level. We observed two important mechanisms involved in chemical depolymerizations with chosen ionic liquids. They disentangle polymers and extend chemically unstable bonds; the one was strongly observed for PET and the other for Nylon-6. Clear observations of both phenomena depend on each ionic liquids. With appropriate thermal input, ionic liquids make the depolymerization process more energy-efficient due to their catalytic characteristics.