Density Functional Theory Studies on Degradation of Polymer Filter for Desalination

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Nanofiltration membranes, which have a tolerance at low pH condition, have been in demand for applications including the removal or recycling of various acids and other valuable chemicals. We investigated the acid-tolerances of aliphatic-amine based and aromatic-amine based polyamide membranes, which have been widely synthesized, using density functional theory (DFT) by calculating the reaction mechanism of acid-catalyzed hydrolysis. In the first step of acid-catalyzed hydrolysis reaction, we observed that amide monomers become twisted by the protonation of oxygen or nitrogen in amide bond. Remarkably, this twist angle (τ) was directly correlated with the energy barrier of the rate determining step (RDS). This is because the τ is related to the delocalization of electrons between the carbonyl πCO bond and nitrogen lone pairs, which determines the stability of the amide bond. This theoretical study suggests that the aromatic membranes exhibit superior tolerance to acid condition than aliphatic membranes due to the lower twist angle of the protonated monomer.