Effect of the difference in terminal halogen atoms on the spontaneity of SPAES polymerization

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Polymer synthesis is a traditional method of material development that depends on researchers' experience. That's why it takes a lot of time and money. Based on quantum mechanics, DFT; density functional theory can be chemically simulated through the computational simulations to investigate the polymerization process thermodynamically. It can improve the traditional methods. In this study, the polymerization process of SPAES; Sulfonated poly(arylene ether sulfone) used as electrolyte polymer is predicted by the first-principle calculation method and the feasibility of simulating polymer synthesis is verified through experiments. SPAES is used as a hydrocarbon-based polymer electrolyte membrane for fuel cells and is prepared by condensation polymerization. Chlorine(Cl) or fluorine(F) is used as terminal atoms of sulfone monomers. Generally, we believe that the synthesis with fluorine (F) is better, but there is no clear explanation yet. Thus, we try to reveal the effect of differences in halogen atoms at the end of monomers on polymerization spontaneity by a computational simulation.