Computational Investigation on Morphology Tunability of Polyimide Microparticles Synthesized via Hydrothermal Polymerization

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Novel synthesis of polyimide microparticles (PIMs) using mellitic acid and three isomers of phenylenediamine (*o*-, *m*-, and *p*-PDA) was conducted via one-pot hydrothermal polymerization. Distinctions in chemical composition and morphology between PIMs were found with the types of PDA isomers, and the C-N bond rotation in amide and imide groups of PIMs was predicted to contribute these differences. With studies of the molecular dynamics simulation and density functional theory calculation, we found that the facile free rotation of the C-N group in imides allows for the formation of spherical morphology in PIM, while the limited rotation in amides does afford the limited degree of freedom. Thus, we anticipate that the relative ratio of amide and imide groups influenced the rotational freedom of polymeric chain segments, and ultimately, lead to the difference in morphology of the respective PIMs.