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Study on the Properties of Biodegradable Polyesters Using Computational and Physical Simulations YEONWOO CHOI, Korea International School, Jeju, RICHARD KYUNG, CRG-NJ — Polymers and plastics have been greatly expanded the many roles they play in the modern industrial economy. However the accumulation of polymeric micro-particles and polymer-based drug carriers in out body can be a significant health risk. A major disadvantage of many Polymers and plastics is their poor biodegradability, which limited their potential applicability in many areas including pharmaceutical uses. In this research, computational methods employing quantum chemistry were used to model various polyesters for their biodegradability and biocompatibility. To measure their effectiveness, the molecules were assessed for thermodynamic stability, reactivity, and polarization. To figure out the structural effect, aliphatic polyesters were first studied for their thermodynamic stabilities and biodegradability, which were measured through the optimized energies. Aliphatic polyesters have been widely used due to their biodegradability and biocompatibility. Also, aromatic polyesters which has excellent material properties but proved to be resistant to microbial attack, were studied for their thermodynamic stabilities and biodegradability. Many aliphatic polyesters turned out to be thermodynamically less stable so they are easily biodegradable.

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