Understanding the Role of Glycerol in a Biodegradable Plastic

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With single-use plastic accumulating and damaging the environment, new and sustainable solutions must be found. One way to do so is using chitosan, found in shrimp shells, and glycerol, a commonly used additive and plasticizer. Though many polyols can be used as plasticizers, using glycerol creates a plastic with the best properties, e.g. flexibility. The reasons for this are not completely understood. Density Functional Theory (DFT) can be used to gain an atomic level understanding of how polyols interact with the chitosan monomer, glucosamine, to design better plastics. This study focuses on glycerol, 1,2 and 1,3 propanediol, and ethylene glycol. First, optimization and frequency calculations were performed on different patterns of two glucosamine (gluc) molecules interacting with two polyol (poly) molecules: poly-gluc-gluc-poly, gluc-poly-poly-gluc, and alternating gluc-poly. We then examined the characteristics of the lowest energy structures. It was previously hypothesized that glycerol was the optimal plasticizer for chitosan because it forces the glucosamine to aggregate, a pattern that is supported by computational evidence. We find that terminal hydroxyl groups are more involved in keeping the structure intact, while middle hydroxyl groups strengthen the intermolecular forces. Therefore, 1-2 and 1-3 propanediol resulted in less stable structures. Currently, we are exploring ab initio molecular dynamics, which could provide a holistic view by introducing greater numbers of glucosamines and polyols. This would give a better idea of the overall structure, rather than the individual interactions between molecules.