Coarse grain simulations of PEG hydrogels

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Cancer immunotherapy, which involves the utilization of T cells to enhance anti-tumor immunity, has demonstrated considerable potential. A significant challenge is to achieve effective expansion and activation of antigen-specific T cells in vitro. Polymeric hydrogels can be functionalized to recruit T cells and promote their expansion and activation. In this regard, hybrid hydrogels integrating synthetic polymers (e.g. polyethylene glycol, PEG) have attracted considerable attention due to their tunable mechanical properties, controllable degradation, and low cost. However, the majority of studies remain experimental relying on trial-and-error approaches, and the structure-property relationships of these hydrogels are unclear. As a "computational laboratory", molecular simulation provides access to the real time molecular scale dynamics of materials' link between microstructure and macroscopic performance. In this work, we consider a coarse grain (CG) implicit solvent model for molecular dynamics (MD) simulations of PEG polymers and hydrogels using the LAMMPS code. In this model, each CG bead represents a C-C-O unit. The force field includes Lennard-Jones interactions, along with bond, angle, and dihedral potentials with parameters adjusted to approximately fit the radius of gyration of PEG chains in implicit solvent. We consider the formation of hydrogels from different concentrations of a star-PEG melt (simulated explicitly by including a reaction step in the MD simulations), followed by equilibration and analysis of its structural and mechanical properties. This study aims to enhance the comprehension of the interactions between such polymers and T cells in molecular level, thereby providing fundamental data and theoretical support for designing PEG-based hydrogel systems for immunotherapeutic applications.

Keywords:
PEG-based hydrogel; Coarse grain models; Molecular dynamics simulations