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Using Atomistic Molecular Dynamics Simulations to Guide Development of Coarse-Grained Models of Polyethylene glycol (PEG), Elastic-like peptides (ELP) and Collagen-like peptides (CMP) For Biomaterial Design FRANCESCA STANZIONE, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE 19716., ARTHI JAYARAMAN, Department of Chemical and Biomolecular Engineering, Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716. — Molecular dynamics (MD) is a well established technique to study the structure and dynamics of biomolecular systems. While atomistic simulations maintain chemical details, they are computationally intensive, thus limiting the accessible time, the length scales and the sampling. To overcome these limitations, coarse-grained (CG) models have proven to be successful in reproducing experimentally relevant length and time scales with reasonable computational expense. CG models can be developed to be phenomenological by effectively reproducing experimental results or can be developed by mapping rigorously to structural information provided by atomistic MD simulations. The latter method is recommended for biomolecules and biomaterials since atomistic simulations capture the detailed effect of the medium on interactions that affect the structure, dynamics and functional properties of the biomolecules, and that can be programmed into the CG models. In this poster we highlight three different cases where atomistic MD simulations provide such essential information to guide CG models: Polyethylene glycol, Elastic-like peptides and Collagen-like peptides based biomaterials.

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