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Multiscale Simulation of polyethylene oxide: Combined United Atom and Coarse-Grained Modeling PRAVEEN DEPA, JANNA MARANAS, The Pennsylvania State University — We present combined united atom [UA] and coarse-grained [CG] molecular dynamics simulations of polyethylene oxide [PEO]. A hybrid region is used to connect united atom and coarse-grained regions, allowing them to occupy different spatial locations in the same simulation box. The presence of a hybrid region allows for a smooth and continuous change in the description of an interacting particle from a coarse-grained bead to a united atom and vice versa. This multiscale simulation is tested with united atom PEO and a coarse-grained model of PEO developed in our group. In the coarse-grained model each CG bead consists of six united atoms and the interactions between them are parameterized to accurately represent static properties, defined by the UA simulations and verified by experiments. Employing the hybrid region in the multiscale simulation works well, as evidenced by good agreement between static properties from the multiscale simulation with those from all UA and all CG simulations. We investigate the performance of the multiscale simulation when addressing dynamics properties, by comparing to UA and CG simulations, and experiments.

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