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Comparison between united atom and explicit atom models for simulation of poly(ethylene oxide) CHUNXIA CHEN, JANNA MARANAS, VICTORIA GARCíA SAKAI, Penn State, JEFFREY LYNN, INMACULADA PERAL, JOHN COPLEY , NIST, PENNYLVANIA STATE COLLEGE TEAM, NIST CENTER FOR NEUTRON RESEARCH TEAM — We compare static and dynamic properties obtained from three simulation models with neutron scattering data for poly(ethylene oxide). The three models are a united atom (UA) model [CH_2 and CH_3 groups are considered as a single unit], the UA model with hydrogen atoms replaced afterwards (UA+H) and an explicit atom (EA) model [all the hydrogens are taken into account explicitly]. Both EA and UA+H models accurately describe the structure as measured via neutron diffraction. If the hydrogen atoms are not replaced in the UA model, the intermolecular peak is still modeled accurately, while the intensity for the intramolecular peak is much weaker than experiments. Dynamically, hydrogen motion in the EA model closely follow the experimental results. The mobility on the UA model is greater than that of carbon and oxygen atoms in the EA model. Since the size of the increase is comparable to the difference in mobility between hydrogen and carbon oxygen atoms in the EA model, the mobility of united atom is approximately equal to that of hydrogen in EA model.

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