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Molecular dynamics simulations of Poly (Ethylene Oxide) and Poly (Propylene Oxide) Aqueous Solutions as a function of temperature. OLEG STAROVOYTOV, DMITRY BEDROV, OLEG BORODIN, GRANT SMITH, Department of Materials Science and Engineering, University of Utah — Molecular dynamic (MD) simulations of aqueous solutions of poly (ethylene oxide) (PEO) and poly (propylene oxide) (PPO) have been performed using polarizable and non-polarizable force fields. Systematic investigation of thermodynamic and structural properties in PEO/water, PPO/water and PEO/PPO/water solutions as a function of temperature have been conducted and compared with available experiments. Our investigation indicate that polarizable force fields perform better in capturing saddle changes in structural and thermodynamic properties of these solution as a function of temperature and therefore represent a better basis for parameterization of temperature-dependent coarse-grained implicit solvent models.

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