

Abstract Submitted
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A Polarizable Potential for Poly(ethylene oxide) in Aqueous Solution OLEG STAROVOYTOV, The University of Utah, OLEG BORODIN, DMITRY BEDROV, GRANT SMITH — We have developed a quantum chemistry-based polarizable potential for poly(ethylene oxide) (PEO) in aqueous solution based on the APPLE&P® polarizable ether and SWM4-DP polarizable water model. Ether-water interactions were parameterized to reproduce the binding energy of water with 1,2-dimethoxyethane (DME) determined from high-level quantum chemistry calculations. Simulations of DME/water and PEO/water solutions at room temperature using the new polarizable potential yielded thermodynamic and transport properties in better agreement with experiment than previously published polarizable and non-polarizable potentials. The predicted miscibility of PEO and water as a function of temperature was found to be strongly correlated with the predicted free energy of solvation of DME in water for the various force fields investigated. Simulations of PEO/water solutions confirm the ability of the new potential to capture, at least qualitatively, the LCST behavior of these solutions

Oleg Starovoytov
The University of Utah

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