

Structure and Dynamics of Poly(urethane-urea) from Molecular Dynamics Simulations

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Abstract: Polymer based membranes for gas capture and separation have been investigated as alternative to the conventional systems, mainly in processes applied by petrochemical and refinery areas [1]. Due to their versatility, poly(urethane) (PU) and poly(urethane-urea) (PUU) have been studied as good candidates to be applied on gas capture/separation [2,3]. Molecular dynamics (MD) simulations not only give support to the experiment, but also can predict structural, dynamical and thermodynamic properties. In this work, a new approach for the point charge model development for polymers simulations is performed, based on a sampling of the conformations and DFT calculations. The intramolecular force field is based on the GAFF parameters using Antechamber and ACPYPE tools. This methodology has been used to generate the topology and subsequent validation by molecular dynamics simulations, using as reference the density and the structure of the pure PUU. The density average obtained in the simulations with a value of 1.06 g.cm^{-3} agrees with data from the literature [4]. Structural calculation by the radial distribution function (RDF) allowed the characterization of microphase separation. The model developed for PUU proved to be satisfactory to represent the studied systems and promising for future works involving polymer membrane simulation.

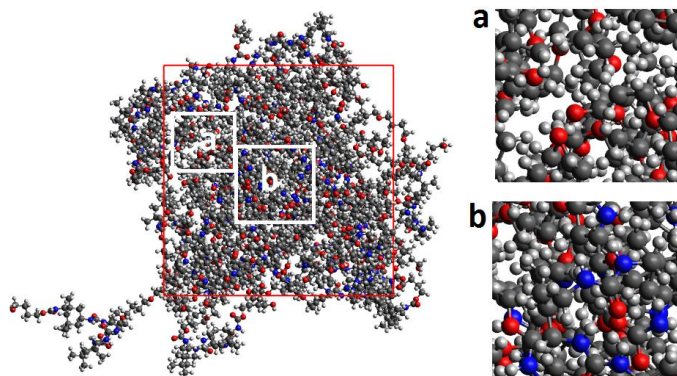


Figure 1 - System framework demonstrating a micro-phase separation

Key-words: polymer, molecular dynamics, simulation, gas separation



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