

Title: A comparative study of the structural analysis of Polymethylene oxide (PMO), Polyethylene oxide (PEO) and Polytrimethylene oxide at above and below T_g by Molecular Dynamics Simulation

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Atomistic molecular dynamics simulations are carried out for poly(methylene oxide) (PMO) and poly(trimethylene oxide) (PTMO) using all atom force-field with the primary objective of comparing the structural details of these two polymers and with available data on poly(ethylene oxide) (PEO). Simulations are carried out at temperatures above and below T_g to investigate the glassy and melt states. Five independently generated amorphous high molecular weight samples consisting of chains of 100 repeating units are simulated for PMO and PTMO. Simulated samples are analyzed for molecular physical structure and thermodynamic properties. Structural analysis includes mean-squared radius of gyration, mean-squared end-to-end distance, dihedral distribution, angle distribution, intrachain and interchain radial distribution functions, intrachain bond orientation correlation function and free volume as a function of temperature. Dihedral angle distribution does not change significantly with increase in temperature, in agreement with results in literature [1]. The simulated data of mean-squared radius of gyration ($<R_g>$) and end-to-end distance ($<R>$) shows that the chain expands with increase in temperature [2]. PTMO chains shows greater expansion with temperature than PMO chains. Solubility parameter (δ) values at all temperatures are found to be in good agreement with literature data. PMO shows higher value of solubility parameter at all temperatures as compared to PTMO. The calculated free volume of these polymers is in the range observed for chemically similar polymers from data available in literature. Free volume for PTMO is higher than that of PMO. Trends shown for the variation of free volume, solubility parameter with temperature are as per the trends reported in literature [3-4]. The results of conformational dynamics as a function of temperature will also be presented for the polymers.

References

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Biography

Sanjeet Kumar Singh has completed his M.Tech from National Institute of Technology (NIT) Rourkela and is currently pursuing his PhD from Indian Institute of Technology (IIT) Madras.

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