

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Tacticity Effects on the Local Conformation and Interfacial Properties of poly (methyl methacrylate) at the Liquid-Vapor Interface KSHITIJ C. JHA, HE ZHU, ALI DHINOJWALA, MESFIN TSIGE, Department of Polymer Science, The University of Akron — The orientation of functional groups of poly (methyl methacrylate) (PMMA) play a key role in understanding functionalities like wettability, aggregation and solvent interaction. We have studied the orientation of different functional groups such as the α -methyl, ester methyl, methylene and carbonyl groups of the PMMA chain through all atom Molecular Dynamics (MD) simulations for different chain lengths of the polymer. Through orientational correlation, and number density computations we are able to establish the identity and extent of groups coming to the surface. Surface tensions are computed to validate our PMMA model. Analysis has been carried out for all three tacticities- atactic, syndiotactic, and isotactic. Sum Frequency Generation (SFG) spectroscopy also provides insight into the orientation of various groups at the liquidvapor interface. Characterization of the SFG peaks is the point of some debate and MD simulations aim to aid in the understanding of local ordering.

Kshitij C. Jha
Department of Polymer Science, The University of Akron

Date submitted: 09 Nov 2012

Electronic form version 1.4