

Abstract Submitted
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Molecular structure of poly(methyl methacrylate) surface: Combination of interface-sensitive infrared-visible sum frequency generation, molecular dynamics simulations, and ab initio calculations¹ HE ZHU, KSHITIJ C. JHA, RAM S. BHATTA, MESFIN TSIGE, ALI DHINOJWALA, Univ of Akron — The chemical composition and molecular structure of polymeric surfaces are important in understanding wetting, adhesion, and friction. Here, we combine interface-sensitive sum frequency generation spectroscopy (SFG), all-atom molecular dynamics (MD) simulations, and ab initio calculations to understand the composition and the orientation of chemical groups on poly(methyl methacrylate) (PMMA) surface as a function of tacticity and temperature. The SFG spectral features for isotactic and syndiotactic PMMA surfaces are similar and the dominant peak in the spectra corresponds to the ester-methyl groups. The SFG spectra for solid and melt states are very similar for both syndiotactic and isotactic PMMA. In comparison, the MD simulation results show that both the ester-methyl and the α -methyl groups of syndiotactic-PMMA are ordered and tilted towards the surface normal. For the isotactic-PMMA, the α -methyl groups are less ordered compared to their ester-methyl groups. The backbone methylene groups have a broad angular distribution and on average tilt along the surface plane, independent of tacticity and temperature. We have compared the SFG results with theoretical spectra calculated using MD simulations and ab initio calculations.

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He Zhu
Univ of Akron

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