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Understanding the Behavior of Poly(3-hexylthiophene) at Liquid/Vacuum Interfaces[1] YENENEH YIMER, MESFIN TSIGE, Department of Polymer Science, University of Akron, Akron, Ohio — Among semiconducting polymers used in opto-electronic devices, poly(3-hexylthiophene) (P3HT) is one of the better candidates because of its good electrical properties and ease of processing. The performance of these devices strongly depends on the structural, morphological, dynamic and interfacial properties of P3HT. Using molecular dynamics simulation and utilizing two different models - all-atom and united-atom - we have studied the dynamic and structural properties of free-standing P3HT thin films at liquid/vacuum interfaces. To quantify these properties, the temperature and chain-length dependence of surface roughness, interfacial width, surface tension, torsional defects, and several other surface properties have been investigated. The results we obtained from all-atom and-united atom models are in reasonable agreement.

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Yeneneh Yimer
Department of Polymer Science, University of Akron

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