

Abstract Submitted
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Molecular Dynamics Simulations of Polymer Surfaces THOMAS CLANCY, SARAH FRANKLAND, National Institute of Aerospace — Due to the increased use of polymer based materials in aerospace adhesive applications, the issues of molecular structure effects and contamination at interfaces have become critical. Computational modeling is being developed to study these systems, with the dual goals of elucidating mechanisms of degradation and developing insights into key structure-property relationships both of which contribute to enabling the prediction of adhesive bond failure. Atomistically detailed models of polymer surfaces, interfaces and bulk structures are constructed and analyzed for this purpose. These models are built with a controlled distribution and content of water molecules to assess the effect of moisture ingress on relevant properties of interest. The models are analyzed and compared to study the effect of moisture on surface and interfacial properties which may influence adhesive bonding characteristics.

Thomas Clancy
National Institute of Aerospace

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