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Molecular Dynamics Simulations of Adhesion at Epoxy Interfaces SARAH-JANE FRANKLAND, THOMAS CLANCY, National Institute of Aerospace, THOMAS GATES, NASA-LaRC — With composite materials becoming more prevalent as metal parts are being replaced on aircraft, adhesives are being developed for composite bonds which are suitable for the various thermal, mechanical and environmental changes that take place over the lifetime of the aircraft. The key molecular structure-property relationships that enable the chemical compatibility of the adhesive with the adherend can be identified with molecular dynamics simulation (MD). MD can assess the role of different chemical moieties in the adhesive, and their behavior in the presence or absence of solvents under different thermo-mechanical conditions. In the present work, MD simulations are used to calculate factors that affect the work of adhesion with and without solvent present. MD simulations are carried out at the interface between components of epoxy-based adhesives and composite adherends. The simulations utilize molecular models of networks which are representative of specific chemistries of the epoxy system. The simulations include both bulk and interface models of the components. The paper will present the simulation methodology, and the results for the work of adhesion..

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