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Steered molecular dynamics of epoxy-amine reactions in EPON862-DETDA YAE JI KIM, SAMUEL REEVE, ALEJANDRO STRACHAN, Purdue Univ — The combination of steered molecular dynamics (SMD) and Jarzynski's equality have made free energy calculations for simulations of non-equilibrium pulling processes possible. This has been widely studied in protein folding and is now applied for epoxy-amine reactions for the first time using the reactive interatomic potential ReaxFF. This reaction in epoxy EPON862 and curing agent DETDA, commonly used in aerospace composite materials, is investigated in both the gas and condensed phases. The potential of mean force (PMF) is calculated during the simultaneous breaking of the epoxy ring and approach of the amine nitrogen to the terminal carbon. Minimization of the PMF is carried out by varying the timing of the reaction (e.g. delayed approach of C-N), as well as a variation of adaptive SMD via a parallel replica method. This adaptive SMD breaks the reaction into a series of time stages, reducing the necessary number of independent simulations and resulting in more rapid convergence of the PMF. Reaction completion is predicted using various initial geometric and molecular features.

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