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Accelerated Molecular Dynamics of Temperature-Programmed Desorption[1] KRISTEN FICHTHORN, KELLY BECKER, MARIA MIGNOGNA, Penn State University — The most widely used experimental method for quantifying thermal desorption is temperature-programmed desorption (TPD). Despite its extensive use, interpretation of this experiment can still be controversial. A significant difficulty with interpreting TPD is that this macroscopic experiment offers a limited picture of the underlying microscopic kinetic events. In this work, we use accelerated molecular-dynamics to simulate TPD of n-pentane from the basal plane of graphite, in the first atomistic simulations to probe TPD over laboratory time scales. Although the simulated TPD spectra agree with experiment, a detailed analysis reveals underlying kinetic phenomena that contrast the standard experimental interpretation and opens new possibilities for understanding molecular kinetics at solid surfaces.

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