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Accelerated Molecular Dynamics Simulation of Thermal Desorption[1] KELLY BECKER, KRISTEN FICHTHORN, Pennsylvania State University — Thermal desorption has been the focus of much surface science research recently. Alkane desorption experiments on graphite [1] show a prefactor that is constant with chain length, while experiments on magnesium oxide [2] show a prefactor that increases with chain length. We utilize an all-atom model to study alkane desorption from graphite. Transition state theory is used to obtain rate constants from the simulation. Accelerated molecular dynamics techniques are used to extend the simulations to experimentally relevant temperatures. Our results provide an explanation [3] for this seemingly contradictory functionality of the prefactor. We also examine the effect that film structure has on the rate of desorption and the shape of the desorption profile through varying coverage. [1] K.R. Paserba and A.J. Gellman, *J. Chem. Phys.* **115**, 6737 (2001). [2] S.L. Tait et al., *J. Chem. Phys.* **122**, 164707 (2005). [3] K.E. Becker and K.A. Fichthorn, *J. Chem. Phys.* **125,** 184706 (2006).

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Kelly Becker
Pennsylvania State University

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