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Accelerated Molecular Dynamics Simulation of Alkane Desorption KELLY MCLAUGHLIN, KRISTEN FICHTHORN, Pennsylvania State University — Thermal desorption has been the focus of much surface science research. Studies of alkanes on graphite[1] and gold[2] have shown prefactors that are constant with alkane chain length but vary by over six orders of magnitude. Other studies on magnesium oxide[3] and gold[4] show a prefactor that increases with increasing chain length. We have developed an all-atom model to study alkane desorption from graphite. Transition state theory is used to obtain rate constants from the simulation. Accelerated MD is used to extend the desorption simulation to experimentally relevant temperatures. Our results show a prefactor that increases with increasing chain length. We predict that it will become constant as internal conformational changes occur significantly. We examine the effect of desorption environment through varying the alkane surface coverage. 1. K.R. Paserba and A.J. Gellman, *J. Chem. Phys.* **115**, 6737 (2001). 2. S.M. Wetterer et al., *J. Phys. Chem.* **102**, 9266 (1998). 3. S.L. Tait et al., *J. Chem. Phys.* **122**, 164707 (2005). 4. K.A. Fichthorn and R.A. Miron, *Phys. Rev. Lett.* **89**, 196103 (2002).

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