

Abstract Submitted
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Aspects of melting in thin molecular films adsorbed onto a graphite substrate using molecular dynamics simulations CARY PINT, Rice University — This work is conducted in order to study the behavior of very thin (nearly 2-D) films of molecules adsorbed onto a graphite substrate when the film is exposed to temperatures near the temperature-induced melting point. Simulations of both the linear normal alkanes (C_nH_{2n+2}) and perfluorinated alkanes (C_nF_{2n+2}) of different chain lengths indicate that the nature of the melting transition in thin films composed of these molecules are dependent upon features of the molecules themselves, such as their chain length and flexibility. This is due to thermal fluctuations that dominate the behavior of the film prior to the melting point which seem to depend on these molecular features, as well as on aspects of the film- such as the adsorbed solid phase. A picture of melting in (quasi) 2-D films based on “allowed” thermal fluctuations is presented, and is expected to be generalizable to more complex films of molecules on a variety of different solid substrates.

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