

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

**Test of the universality of the scaling energy in alkanes based on the melting transition of monolayers adsorbed on graphite**<sup>1</sup> L. FIRLEJ, Université Montpellier 2, B. KUČHTA, Université de Provence, M. ROTH, University of Northern Iowa, C. WEXLER, University of Missouri — The quality of the results of computational treatment of complex systems depends crucially on the quality of the interaction potentials used. When modeling non-rigid molecules an essential difficulty resides in the correct accounting for all energies related to internal degrees of freedom. Of particular importance is to avoid over- or under-counting non-bonded intramolecular van der Waals and electrostatic interactions between close neighbors that are chemically bonded. In many force fields (e.g. CHARMM) 1-4 non-bonded interactions are scaled down by the use of the “scaling factor” (SF). Typically, this SF is assumed to be universal (and  $\sim 0.5$ ). In this talk, we study this universality hypothesis by comparing computational and experimental melting temperatures of alkane monolayers adsorbed on a solid graphite surface. Three alkanes (C6, C12, C24) of different lengths (7-30 Å) have been analyzed using an all-atom representation, standard CHARMM parameters, and various SF's. We show that the scaling parameter has no universal value but depends on the molecular length.

<sup>1</sup>Support: U.S. DOE (DE-FG02-07ER46411), ACS-PRF (PRF43277-B5), and Univ. of Missouri Bioinformatics Consortium.

Carlos Wexler  
University of Missouri

Date submitted: 08 Dec 2008

Electronic form version 1.4