Test of the universality of the scaling energy in alkanes based on the melting transition of monolayers adsorbed on graphite[1] L. FIRLEJ, Universit Montpellier 2, B. KUCHTA, Universit 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 ~ 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 $\mathring{A}$) have been analyzed using an all-atom representation, standard CHARMM parameters, and various SFs. We show that the scaling parameter has no universal value but depends on the molecular length.

X	Prefer Oral Session
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Carlos Wexler
wexlerc@missouri.edu
University of Missouri

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