Test of the universality of the scaling energy in alkanes based on the melting transition of monolayers adsorbed on graphite

L. FIRLEJ, Université Montpellier 2, B. KUCHTA, 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) 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.

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