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Test of the universality of the scaling energy in alkanes using melting transition of layer adsorbed on graphite

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— The non-bonded terms together with the torsional energy determine the internal (conformational) degrees of freedom of simulated alkanes. Being able to predict the energy and ordering of conformations correctly is an essential quantity for bringing force field methods into the predictive regime of theoretical methods. To estimate the universality of modern force fields it is helpful to know how different components of classical fields affect the simulated properties. In the case of alkanes, the interplay between torsion potential and the scaling of 1-4 van der Waals and 1-4 charge-charge (QQ) interactions plays a crucial role. It is the purpose of this work to study universality of the scaling factor of 1-4 non-bonded interactions in alkanes. Three alkanes of length from 7 to 30Å (C_6, C_{12}, C_{24}), in an all-atom representation have been analyzed.

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