MD Simulations on Fluorinated Alkanes

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Comparing molecular dynamics calculations on clusters of eicosane(ES/128), perfluorinated (PFES/128) and semifluorinated(SFES/128) eicosane have been performed using the AMBER program. The different behaviour of conventional and fluorinated alkanes in the process of molecular aggregation was investigated. Moreover, mixed clusters of decane(DC/92) and perfluordecane(PFDC/92) have been studied by MD simulations. The applicability of the AMBER force field has been verified by comparison with ab initio and PM3 calculations on the isolated PFES molecule.

The flexibility of the chains and the influence of structure formation in the clusters as well as the tendency of microphase separation in the mixtures have been analyzed by snap shots, radial atomic pair distribution functions g(r) and orientation correlation functions g(o) with respect to the corresponding basic atoms and vectors.