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Structure formation of toluene around C60: Application of the Adaptive Resolution Scheme CHRISTOPH JUNGHANS[1], Los Alamos National Laboratory, SEBASTIAN FRITSCH, KURT KREMER, Max Planck Institute for Polymer Research — In the adaptive resolutions scheme (AdResS) a local, typically all-atom cavity is coupled to a surrounding medium of coarse grained, simplified molecules. This methodology cannot only be used to reduce the CPU time demand of atomistic simulations but also to systematically investigate the relative influence of different interactions on structure formation. For this, we vary the thickness of the all atom layer of toluene around a C60, analyze the first toluene layers and compare the result to a full resolution simulation. With this system, we also introduce the implementation of AdResS for molecular simulations into GroMaCS.

[1]Work was performed at the Max Planck Institute for Polymer Research

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