Extension of mesoscopic DPD parameterization to model variable bead volumes and hydrogen bond interactions

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In this talk, we will give an overview of the parameterization of coarse-grained interactions of Dissipative Particle Dynamics (DPD) simulation method[1, 2]. DPD is a useful tool to simulate various soft materials including polymers, surfactants, bilayers. DPD parameters are often mapped from thermodynamic quantities, which makes DPD a straightforward tool to be applied to different materials. In the conventional DPD framework, DPD beads are considered as having similar bead volumes. However this assumption, if applied to a real polymer, might lead to an incorrect meso-structure since real beads might differ in volume. To propose a solution to this drawback, we introduce an alternative parameterization of DPD where bead volumes are different and dictated by their pure-liquid volumes[3]. To extend the application of DPD to polymers near hard surfaces, a dual-scale parameterization approach is put forward. By these parameterization approaches, we simulate a widely used polymer, an epoxy, in bulk [4] and next to a metal-oxide surface [5, 6]. Most of the polymeric materials expecially in biomedical area involve hydrogen bond interactions. Modeling the attraction coming from the hydrogen bond interactions in DPD is crucial to create the correct equilibrium structure of such materials. In the final part of the talk, we will address the recent parameterization of DPD where an attractive term is added to the conservative DPD potential which represents the hydrogen bonds [7], and its application to hydrogels.

References

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