CHAPTER IV
CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

All-atom molecular dynamics simulations were performed for elucidating the aggregate morphology of aqueous SDBS surfactants adsorbed on (6,6), (12,12), and (20,20) SWNTs. The effect of surface coverage and SDBS molecular structure were investigated. Because of computing limitations, relatively low surface concentrations were considered. Simulation results show that the self-assembly of SDBS molecules depends on the surface coverage, as well as the SWNT diameter. Changing the SDBS molecular architecture affects the surfactant arrangement on the nanotubes. The results are quantified using representative simulation snapshots, density profiles away from the nanotube surfaces, and orientation probability maps.

Both surfactants tend to yield disordered aggregates on all the simulated nanotubes. Linear SDBS, especially at low surface coverages, tend to orient parallel to the (6,6) SWNT axis because of the relative rigidity of the surfactant tail and the small diameter of the nanotube. At low surface coverages, the linear SDBS adsorb via both surfactant tail and benzene ring on the nanotube surface. As the surface coverage increases, the surfactant tails protrude extensively towards the aqueous phase, effectively pulling the benzene rings present within SDBS away from the nanotube surfaces.

The morphology of self-assembled aggregates formed by branched SDBS surfactants appears to depend more significantly on the SWNT diameter than those obtained for linear SDBS, especially at low coverages. Specifically, the branched SDBS simulated appears to be compatible with the curvature of (6,6) SWNTs. On all nanotubes considered the branched SDBS tails remain adsorbed onto the nanotube surface, while the benzene rings and the sulfonate group protrude towards the aqueous phase.

These results show that it is possible to manipulate the morphology of self-assembled surfactant aggregates on SWNTs by tailoring their molecular architecture.

Based on calculations for the effective potential of mean force between carbon nanotubes in aqueous surfactant systems available in the literature, it appears that by controlling the morphology of the surfactant aggregates will lead to the selective stabilization of aqueous carbon nanotube dispersions.

5.2 Recommendations

Several recommendations for future work can be offered, as MD simulation study enhances understanding of the role of surfactants such as SDBS in improving the dispersion stability of individual SWNTs in aqueous solution. It is possible to carry out the simulations to compute the potential of mean force (PMF) between two parallel SDBS-coated SWNTs as a function of intertube separation, in order to shed new light on the dispersion on the dispersion and stability mechanism of SWNT in aqueous SDBS solution.

Because SDBS surfactants are composed of various molecular architectures, it is interesting to simulate aqueous SDBS surfactants adsorbed on SWNTs by varying either the number of carbon atoms in the SDBS alkyl tails (e.g., 1 to 16) or the position of attachment of the benzene ring on the alkyl chain. Moreover, to further study a mixed system of surfactants (e.g., 50% of linear and 50% of branched SDBS), could be performed leading to a better understanding the adsorption and the self-assembly of SDBS on SWNTs.