CHAPTER V
CONCLUSION AND RECOMMENDATIONS

DPD simulation of SDS aggregation on different graphene surfaces was performed. From the results, two conclusions can be drawn. Firstly, aggregate orientation, order parameter, and density profiles suggest that size, shape, and composition of carbonaceous surfaces affect the orientation of the surfactants and aggregate morphology. On both sheets and nano-ribbons, the aggregate tends to be multi-layered hemi-micelle when the sheet size is small, and gradually becomes mono-layered, as the size or the width of the nano-particle increases. The presence of oxide edges restricts the aggregate from moving from one side to another side, keeping the amount of surfactants on both sides constant, and also condenses the aggregate within the boundaries. The aggregate restriction can reduce the exposure of nano-particle to another nanoparticle, with optimum amount of SDS. The mechanism of GS agglomeration was also studied. The results suggest that the sheets tend to agglomerate when the amount of surfactant coverage is low. However, the different outcome between the cases with same coverage has implied that the different arrangement of aggregate and the amount of surfactants present on different GS, as studied earlier, does matter in the agglomeration process, but the fact that lower surface coverage leads to higher possibility of agglomeration remains true. The size of the GSs is also assumed to be another factor that leads to different approaches of agglomeration, as we study from the record of agglomeration times. With these studies, one can gain the insight of the agglomeration mechanism and learn to prevent it with optimum size of the nano-particles and amount of surfactants used, or manipulate it to produce nano-particles of desired dimension. The knowledge obtained here can be useful for optimizing the dispersion of graphitic nano-fillers in the nano-composite material production. What remain unknown in this simulation are the results of the same simulation, in larger simulation space and longer period of time, since certain phenomena require much longer time to occur.