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Coarse-Grained Force Field Development of Novel Bolaamphiphilic Molecules: VOTCA or Martini?[1] BIJAY SHRESTHA, HYE-YOUNG KIM, Southeastern Louisiana University — We have performed a series of atomistic molecular dynamics (MD) simulations of novel bolaamphiphilic molecules, VECAR, in water in recent years. At low molar density, the VECAR molecules aggregate in water to form small-size micelles which have a potential application as a drug-carrier. With the atomistic MD simulation results, many data analyses were carried out to understand the structure of the self-assemblies and the dynamic process of the aggregation in the atomistic level. However, to be able to study the interactions of the micelle with other micelles or a lipid bilayer membrane in a biophysical environment, we need to use coarse-grained (CG) molecular dynamics simulations. We have developed CG force fields of the novel molecule using both VOTCA and Martini methods. The summary of our findings and the comparisons of using the structure-based method (VOTCA) and free-energy-based method (Martini) will be presented.

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