The Effect of Alkylation on Chemical Structure and Bulk Property of Graphene Oxide

이민환, 권상우, 이원보†
서울대학교
(wblee@snu.ac.kr†)

The graphene oxide(GO) could processed into bulk scale materials with layered structure. For realistic modeling of the materials the molecular structure of graphene oxide and its alkylated derivatives were modeled considering formation energy of functional groups and reaction energy of alklataion to estimate ratio of each chemical groups. The adsorption number of alkyl chains on graphene oxide was analyzed by grand canonical monte carlo (GCMC) simulation where the number of adsorbed chains. With realistic structure of AGOs the layered structure was derived by molecular dynamics simulation from which the distance between layers were calculated. Due to the multiscale modelling the relationship between bulk property and chemical structure was investigated.