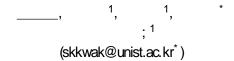
Water droplet simulation on graphene grafted with various functional group



Assessment of the amount of defects and their types of graphene is important for its various applications, whether it is physical or chemical. Graphene defects that we have studied consist of hydroxyl, epoxy, ether, carbonyl, carboxyl, pyridyl, hydrogen-attached defect, and simple vacancy. On defective graphene with aformentioned types of defects, we analyzed wetting property by contact angle of water in nanoscale via molecular dynamics (MD) study. From obtained contact angles, we found that simple vacancy defect showed higher hydrophobicity than pristine graphene and the C-O and C-N groups showed small contact angle due to hydrophilicity. These results are helpful to verify grade and structural nature of graphene in the first screening stage.