Water droplet simulation on graphene grafted with various functional group

박주현, 봉지혜[1], 주상현[1], 곽상규*
울산과학기술대학교; [1]경기대학교
(skkwak@unist.ac.kr*)

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 aforementioned 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.