

Estimation of Contact angle variation of water droplet on graphene

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Easy and reliable estimation of properties of graphene is crucial for the variety of potential applications of graphene. We characterized the wetting properties of defective graphene using molecular dynamics (MD). Graphene defects were categorized by hydroxyl, epoxy, ether, carbonyl, carboxyl, pyridinic, and hydrogen-attached defects. We confirmed the contact angle of water on graphene varied with the concentration and type of defects. Hydrogen attached defect made graphene more hydrophobic. Other types with oxygen and nitrogen contained defects made graphene more hydrophilic. As the concentration of defect increased, the contact angle was either increased or decreased. However, the contact angle of pyridinic graphene was decreased and slightly increased till being constant. We interpreted the contact angle in terms of the adhesion energy between graphene and water droplet and water layering effect.