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First-order phase transition of temperature-dependent wettability on a graphite surface

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Abstract

In this paper, using molecular dynamics simulation, the wettability dependence of a graphite surface consisting of two layers of graphene on temperature is studied for three water models. For each given temperature, the wettability of the graphite surface is determined by estimating the contact angle of the macroscopic droplet using extrapolation method in terms of inverse radius for water nanodroplets. Although the used models show little wettability at room temperature, the result of our simulations suggests a wetting transition event for all three models studied at temperatures lower than their critical temperature. The observed trend for the dependence of the contact angle on temperature and the approximate value of the transition temperature is comparable to the experimental results recently reported for graphite. Fitting the curves to a proposed model shows that the wetting transition event is first order for all three models.

Keywords: Molecular dynamics simulation, graphene, graphite, phase transition, wettability

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