Water nanodroplets on graphite and graphene - MD insight

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Since the discovery of graphene, a never - ending debate has started in literature about the wettability of its surface. Not only experimental, but also simulation studies have been reported. Among them the study of Werder et al. reporting the force-field for SPC/E water nanodroplets on a graphene is probably on of the most important. However, due to some faults of applied water model, as well as due to insufficient simulation time, the new force-field should be proposed and discussed. We use the TIP4P/2005 water model for this purpose. Considering graphene wettability the influence of a bottom layer rotation on water contact angle is analyzed. Next the problems of HOPG wettability is discussed. So called "switchable" hydrophobicity/hydrophilicity of a HOPG is proved and it is suggested that this phenomenon can be very important from the practical point of view. Finally the Wenzel states of water wetting different HOPG-like models are discussed by Molecular Dynamics (MD) with the special attention to the state of water inside HOPG-like pores.

References

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