***Ab* Initio Calculations of Electrical Structures of Water Adsorbed on Graphene**

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A graphene, which consists of carbon atoms arranged in hexagonal lattice, is well suited for exploring an interaction between a material surface and a molecule. This is because it is an atomically flat and non-polar material. It had long been considered that graphene cannot be adsorbed by water molecules because it is a hydrophobic material. However, the previous molecular dynamics (MD) simulations confirmed that there are single or double water layers on a graphene surface, depending on the number of water molecules [1,2]. Similar layer structures have already been reported for a carbon nanotube by Homma et.al., and they found such layer structures formed around the carbon nanotube by both photoluminescence measurements and classical MD simulations [3]. Although the layer structure perpendicular to a graphene surface has been rigorously researched, the microscopic structure parallel to the surface has not yet been fully characterized, meaning that the hydrogen bonding network in the water layers on graphene is not understood enough. Moreover, the influence of surface water on the electronic states of a graphene remains to be elucidated yet although this is essential for developing of graphene-based devices, such as a graphene field-effect transistor.

In this work, we constructed microscopic structures of surface water adsorbed on a free-standing graphene and a graphene attached on a hexagonal boron nitride substrate using classical molecular dynamics simulations. For the obtained structures, we investigated the influence of surface water on electronic states of a graphene using *ab initio* calculations based on the density functional theory. From the above methods, we clarified that the characteristic polygonal structures appear in the two-dimensional hydrogen-bond network [4]. We present that the structure of surface water and the electronic states of water adsorbed on a graphene.

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