First Principles Analysis of Adsorption Geometry and Electronic Properties of Monolayer Naphthalene on Graphene

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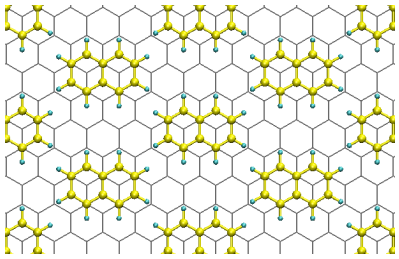

Fig. Monolayer naphthalene on graphene (top view)

The development of molecular-based electronic devices is highly dependent on the knowledge of the interaction between molecules and solid surfaces. By using first principles calculation based on van der Waals density functional method, we aim at a better calculation to understand the interaction between the molecule and the solid surfaces. Naphthalene adsorption on graphene is investigated as a model of interface system. While the intermolecular interaction has not been fully considered in previous theoretical study[1], recent scanning tunneling microscope (STM) measurements of naphthalene on graphite surface[2] suggest that intermolecular interaction plays an essential role at monolayer coverage. Since the geometrical structure of the interface will strongly influence its electronic properties and vice versa, it is important to calculate the geometry precisely. As a result, at monolayer coverage (as shown in figure), the molecule becomes slightly tilted, in good agreement with experimental result by Yamada and co-workers.[2] The tilted configuration results from the balance between intermolecular interaction and naphthalene-graphene interaction. We next investigate the unoccupied states of the adsorbed system and focus on the image potential states (IPSs) as observed experimentally on the naphthalene-graphite interface.[3] The lowest graphene IPS (LGIPS) is hybridized with unoccupied states of the naphthalene layer. We find the IPS-like state appears in naphthalene layer, naphthalene IPSs (NIPSs). This is interesting because IPS usually exist in solid surfaces. Hybridization between the NIPS and the LGIPS then forms the new IPS states. Unlike the effective mass of LGIPS, which is isotropic, the effective mass of the new IPS is anisotropic. This is essentially due to the large anisotropy in the uniaxially oriented naphthalene layer..

Reference

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