Water on Graphene-Coated TiO_2: Role of Atomic Vacancies

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Beyond two-dimensional (2D) materials, interfaces between 2D materials and underlying supports or 2D-coated metal or metal oxide nanoparticles exhibit excellent properties and promising applications. [1] The hybrid interface between graphene and anatase TiO_2 shows great importance in photocatalytic, catalytic, and nanomedical applications due to the excellent and complementary properties of the two materials. [2, 3, 4] Water, as a ubiquitous and essential element in practical conditions and in the human body, plays a significant role in the applications of graphene/TiO_2 composites for both electronic devices and nanomedicine. Carbon vacancies, as common defects in chemically prepared graphene, [5] also need to be considered for the application of graphene-based materials. Therefore, the behavior of water on top and at the interface of defective graphene on anatase TiO_2 surface was systematically investigated by dispersion-corrected hybrid density functional calculations. [6] The presence of the substrate only slightly enhances the on-top adsorption and reduces the on-top dissociation of water on defective graphene. However, at the interface, dissociated water is largely preferred compared with undissociated water on bare TiO_2 surface, showing a prominent cover effect. Reduced TiO_2 may further induce oxygen diffusion into the bulk. Our results are helpful to understand how the presence of water in the surrounding environment affects structural and electronic properties of the graphene/TiO_2 interface and thus its application in photocatalysis, electronic devices, and nanomedicine. [7]

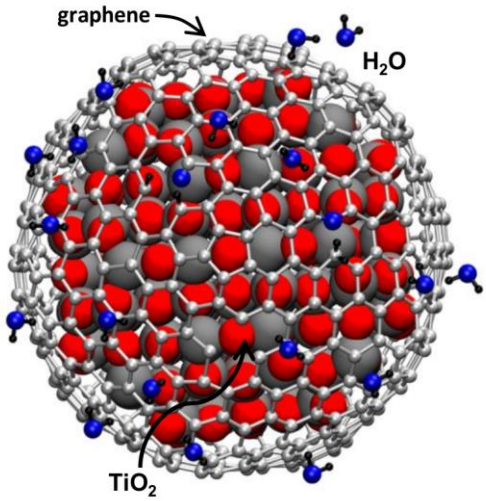

Figure 1: H_2O reactivity with the graphene/TiO_2 interface in the presence of defects.

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