

Catalysis under Cover: Enhanced Reactivity at the Interface between (Doped) Graphene and Anatase TiO₂

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The “catalysis under cover” involves chemical processes which take place in the confined zone between a 2D material, such as graphene, h-BN, or MoS₂, and the surface of an underlying support, such as a metal or a semiconducting oxide [1,2]. The hybrid interface between graphene and anatase TiO₂ is extremely important for photocatalytic and catalytic applications because of the excellent and complementary properties of the two materials [3]. We investigate and discuss the reactivity of O₂ and H₂O on top and at the interface of this hybrid system by means of a wide set of dispersion-corrected hybrid density functional calculations [4]. Both pure and boron- or nitrogen-doped graphene are interfaced with the most stable (101) anatase surface of TiO₂ in order to improve the chemical activity of the C-layer. Especially in the case of boron, an enhanced reactivity toward O₂ dissociation is observed as a result of both the contribution of the dopant and of the confinement effect in the bidimensional area between the two surfaces. Extremely stable dissociation products are observed where the boron atom bridges the two systems by forming very stable B-O covalent bonds. Interestingly, the B defect in graphene could also act as the transfer channel of oxygen atoms from the top side across the C atomic layer into the G/TiO₂ interface. On the contrary, the same

conditions are not found to favor water dissociation, proving that the “catalysis under cover” is not a general effect, but rather highly depends on the interfacing material properties, on the presence of defects and impurities and on the specific reaction involved [5].

References

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Figure

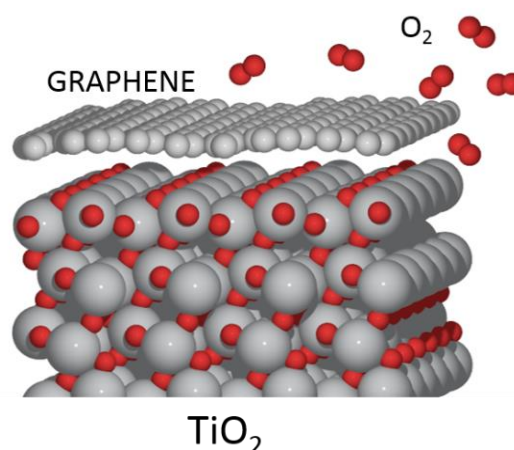


Figure 1: O₂ reactivity on top and at the G/TiO₂ interface.