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Theoretical study on electronic properties of 2D graphene-TiO2 nanocomposites YASUYUKI MASUDA, GIACOMO GIORGI, KOICHI YAMASHITA, Department of Chemical System Engineering, School of Engineering, The University of Tokyo — In recent years, bidimensional graphene-TiO2 nanocomposite materials have attracted deep interest since their potential applicability in photocatalytic and photovoltaics. It is extremely appealing, indeed, the possibility of synthesizing a composite materials able to embody both the semiconducting properties of TiO2 monolayers and the excellent transport ones of graphene.The synthetic path, similarly to the electronic and optical properties of such nanocomposites, is nowadays considered a hot-topic in materials science. However, on the theoretical side, predictive results on the properties of a so promising material with device-oriented relevance are astonishingly very scarce.In this work, we focus on the impact that the mechanical stress at the interface formed by graphene and a monolayer of anatase (001)-oriented exerts on electronic and optical properties of the final nanocomposite. In order to perform such analysis, we have modeled and optimized, by means of Density Functional Theory, several graphene-TiO2 monolayer models, examining and reporting analogies and differences between models in presence and in absence of a direct chemical bond. In this poster presentation, we report the results of these calculations and the predicted electronic properties of these nanocomposites.

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