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A DFT study on the effect of supporting titania on silica graphene epoxy graphene and carbon nanotubes - Interfacial properties and optical response

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ABSTRACT:

A first principles study of the Titania is done as used in photo-catalysis to generate charge carries. Models of titania, silica, graphene, epoxy graphene monoxide, single wall Carbon nanotubes and their respective layer were studied in order to investigate their morphological, electronic and optical properties as well as electrostatic potentials. The calculations are performed using density functional theory to ascertain the properties of the starting bulk molecules and understand the surface properties, a slab surface of 101, and 111 is cut from the bulk TiO2 and SiO2, respectively. A physisorbed study is carried out on the layers generated in relation to their electronic and optical properties. To understand the electron movement during photocatalysis, a projected density of state study is conducted in order to assess the orbital contribution in the charge transfer.