

Simulation from the first principal theory on the effect of supporting silica on graphene and the new composite material

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ABSTRACT:

Silica has been used as support material with many photocatalytic materials. In this study, silica polymorphs on graphene and epoxy graphene were studied using Density Functional Theory (DFT) to determine the interfacial and optical properties of the composite material. The powder diffraction patterns and Raman spectra for the silica polymorph structural models as well as graphene and epoxy graphene monoxide were generated using Material Studio (2016), and the GGA in PBE first principle method. The electronic and optical properties as well as work function analysis of the polymorphs with graphene and epoxy graphene monoxide starting molecules together with the layers systems were compared. In Our findings the optical properties of the layers generated were sensitive to the visible light in both epoxy-graphene monoxide and graphene composites.