The g-C_3N_4/anatase (101) interface for photocatalytic applications: insights from hybrid DFT

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ABSTRACT

Due to the importance of carbonaceous materials such as graphitic carbon nitride (g-C_3N_4) to enhance solar light-driven photocatalytic activity of TiO_2 [1], we present a theoretical investigation of the structural, electronic, and optical properties of a g-C_3N_4/TiO_2 composite and of its S-doped variant. We combine periodic hybrid DFT calculations for all structural and electronic properties to time-dependent DFT (TD-DFT) carried out on finite clusters extracted from the periodic structures and embedded in an array of point charges devised to reproduce the periodic electrostatic environment [2,3]. Our calculations suggest suitable properties of both composites for photocatalytic applications, with distinct contributions of g-C_3N_4 and TiO_2 close to the band gap, highly anisotropic effective masses with low recombination rates of electrons and holes, as well as an enhanced photoabsorption compared to freestanding TiO_2 or g-C_3N_4. The proposed computational protocol, combining both periodic and non-periodic DFT calculations, appears as a reliable and effective tool to model both the electronic and the optical properties of heterostructures at low computational cost.

References

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