Hybrid TiO_2/Graphene Derivatives Nanocomposites: Is Functionalized Graphene Better than Pristine Graphene for Enhanced Photocatalytic Activity?

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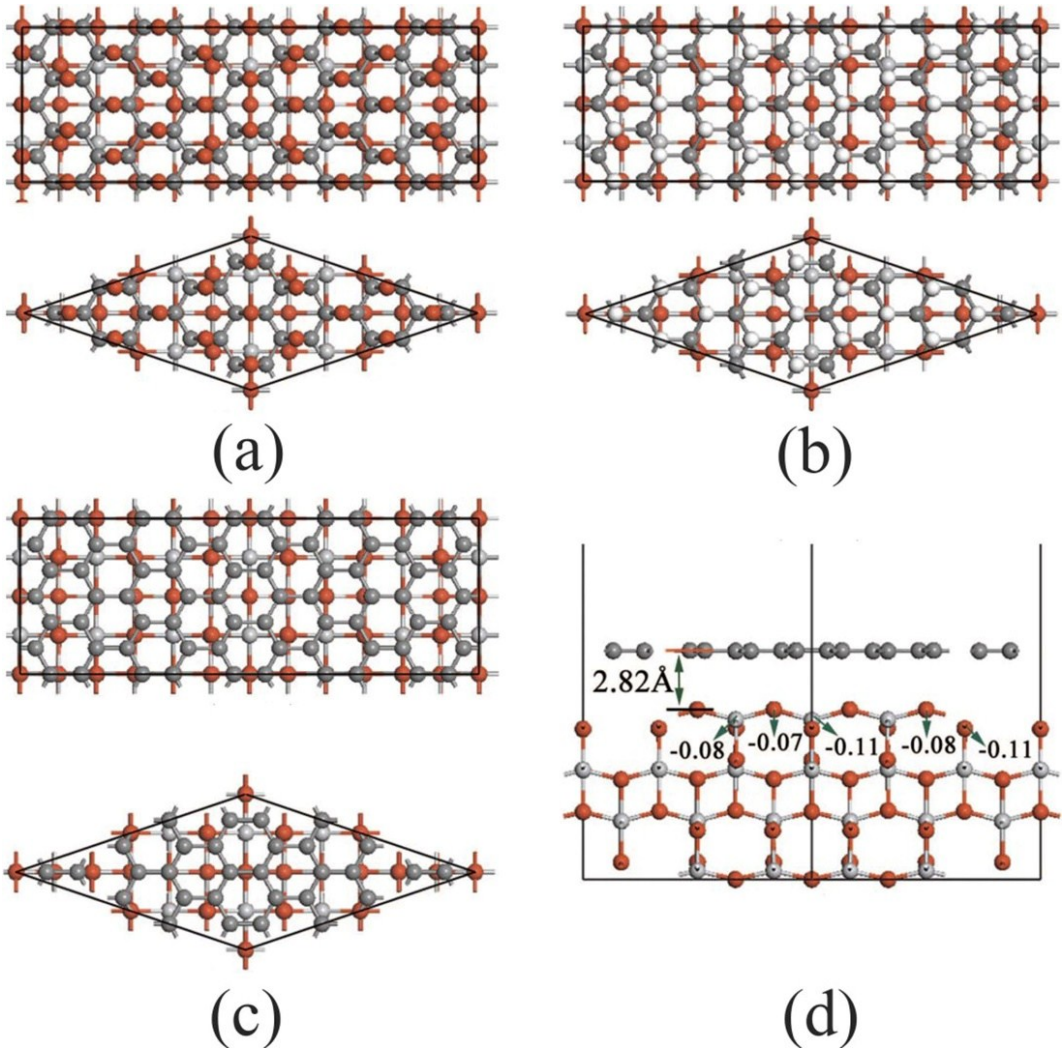

Fig. S1 (a), (b) and (c) for the simulated model of TiO_2/RGO, TiO_2/GRH and TiO_2/GR nanocomposites; top and bottom panels for top view of super cell and top view of primitive unit cell of TiO_2/RGO(GRH, GR), respectively. (d) for the side view of primitive unit cell of TiO_2/GR nanocomposites. Light gray, red and black sphere represent Ti, O and C atoms, respectively. The atoms in the surface layer of TiO_2(001) have a slightly movement, and the positive (negative) values represent the atom slightly move upwards (push downwards).

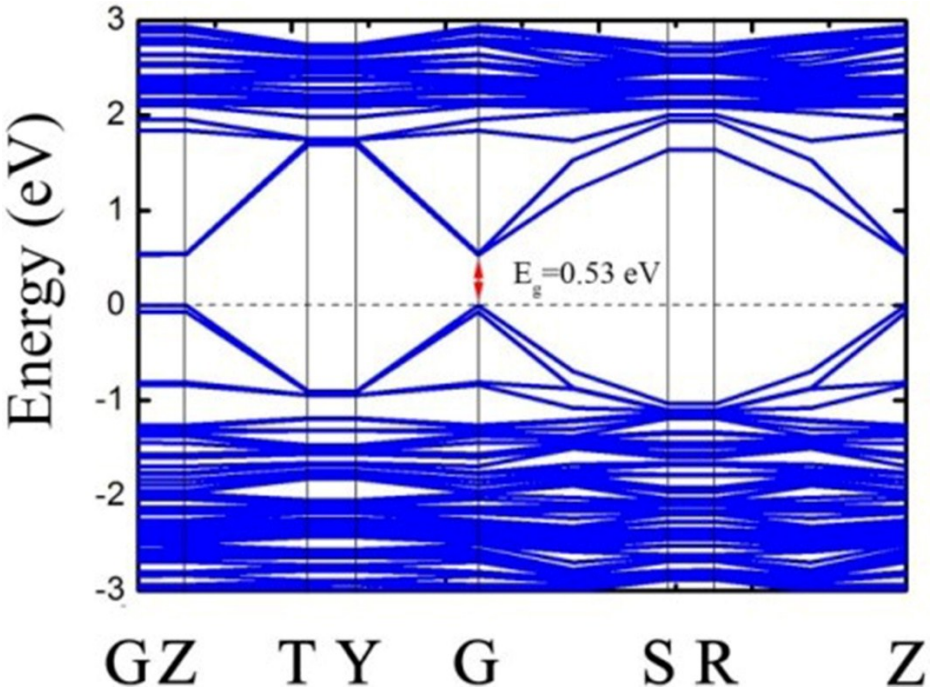

Fig. S2 Band structures for TiO_2/GR. The horizontal dashed line indicates the Fermi level.

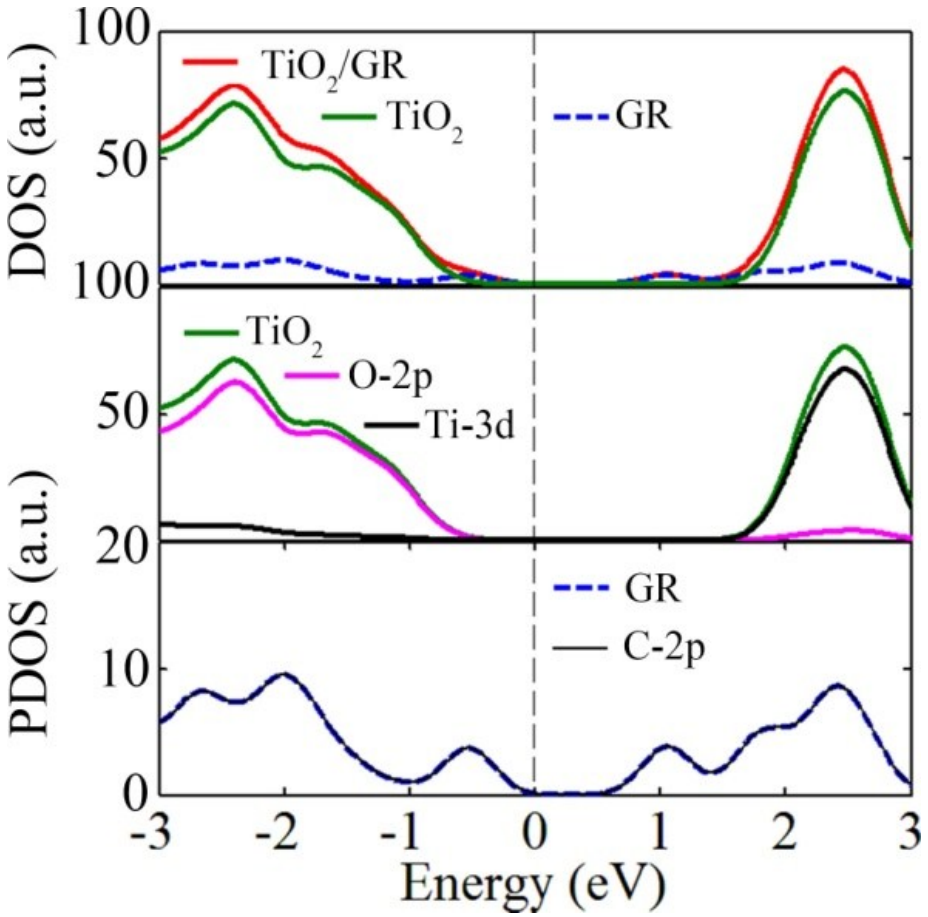

Fig. S3 DOS and PDOS for the TiO_2/GR nanocomposites. Top, middle and bottom panels for DOS, PDOS of TiO_2 component and GR component of TiO_2/GR, respectively. The Fermi level is set to zero.

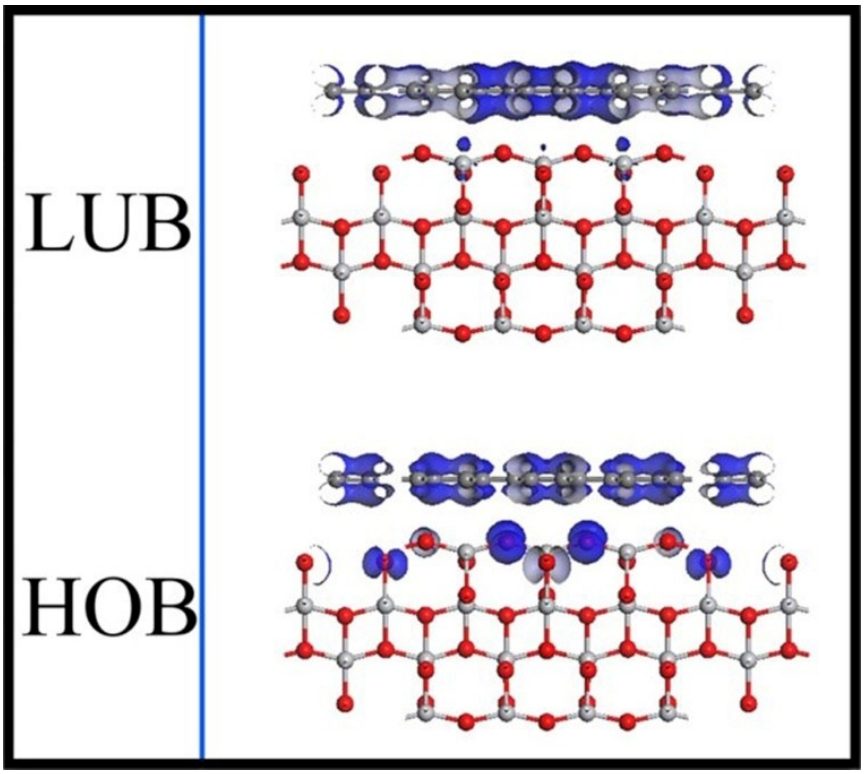

Fig. S4 Maps of the electron and hole density distributions for the HOB and LUB with an isovalue of 0.003 e/Å^3 for the hybrid TiO_2/GR. Here, HOB and LUB denote the highest-occupied and lowest-unoccupied bands, respectively. A type-I heterojunction form on TiO_2/GR nanocomposites.

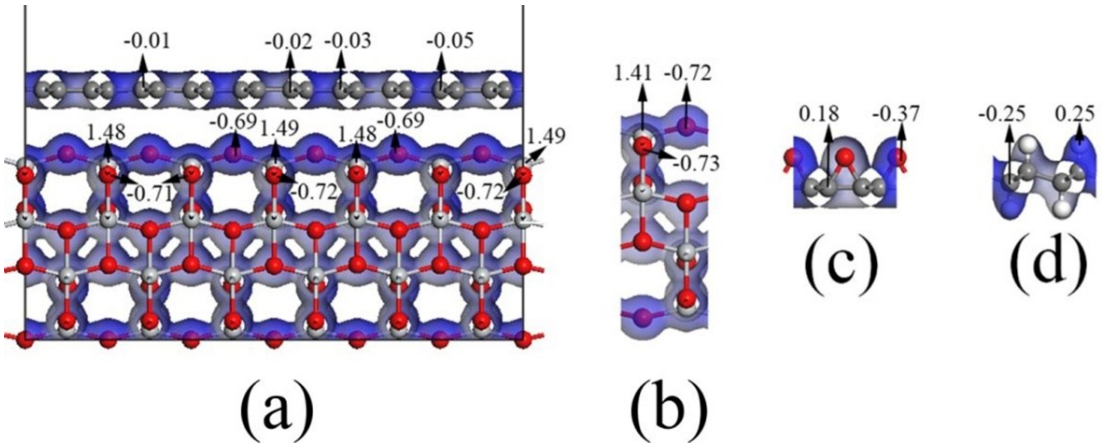

Fig. S5 Charge distribution map of (a) TiO_2/GR, (b) pure TiO_2(001), (c) monolayer RGO and (d) monolayer GRH with a isovalue of 0.4 e/Å^3. Light gray, red, black, and white sphere represent Ti, O, C and H atoms, respectively.