Photocatalytic TiO_2/graphene-based charge-transfer interfaces

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Research question: Explain the high efficiency of TiO2/reduced graphene oxide photocatalysts

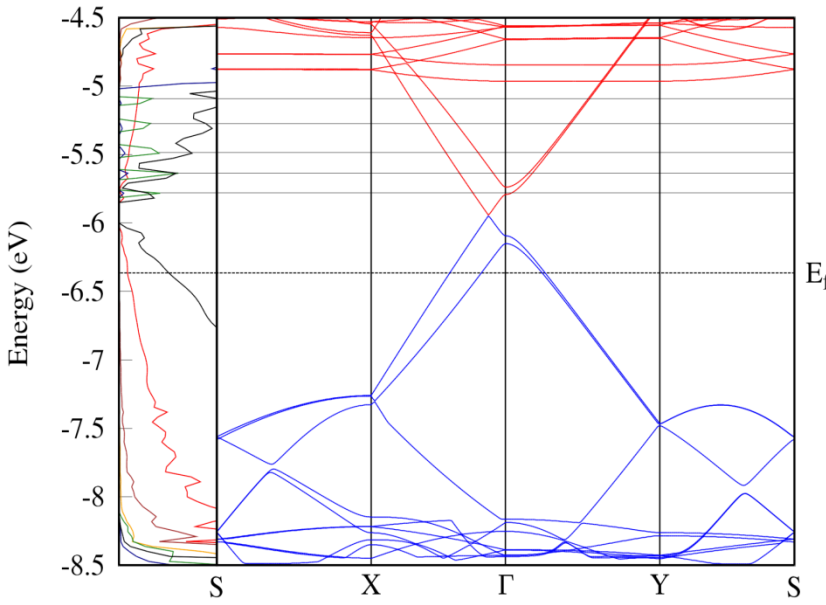
Computational challenges:

- Commensurability => large systems : 180 atoms TiO_2 + 72 atoms C
- Need hybrid functionals to describe TiO_2
- Need dense k-point grid to describe graphene

Our approach:

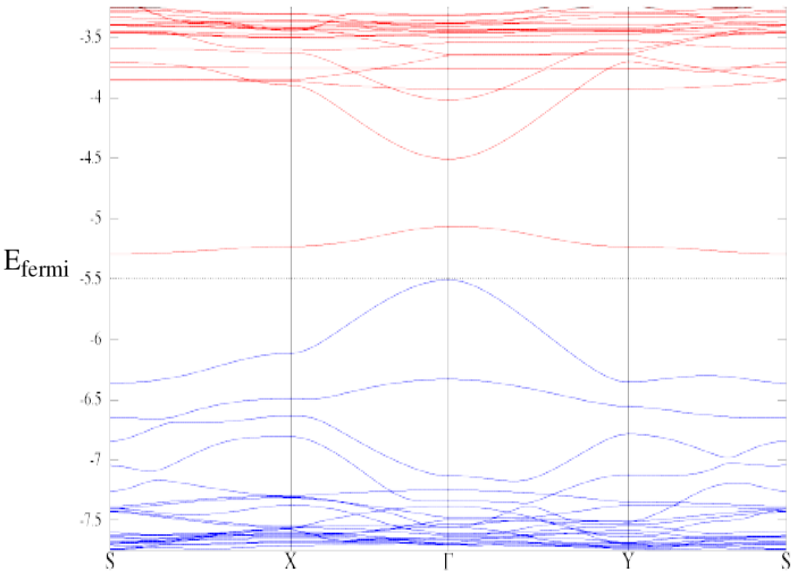
- Geometry optimisation using CP2K (first PBE, then HSE06 using ADMM)
- Electronic structure analysis using CRYSTAL

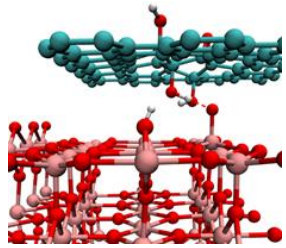
1. TiO_2 (rutile)/graphene



2. TiO_2 (rutile)/reduced graphene oxide (RGO)

RGO model: C:O ratio =12:1;
4 OH, 2 epoxy groups





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