Computational modeling of Doped TiO_2 Thin Film Surface

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Titanium dioxide (100) thin film surfaces are doped with platinum and ruthenium [1]. The formula $E_2Ti_{16}O_{32}H_{72}$ is used, and the (100) crystallographic surface is exposed and covered with a monolayer of water where E is either Pt or Ru. The simulation cell is treated with periodic boundary conditions along X and Y axes, and a vacuum layer of at least 8 Å was added above the upper surface of the slab to avoid spurious interactions between the periodic images of the system. Optimization is completed by DFT and PBE in VASP[2] software. The density of states is compared between slabs doped by the two elements as well as $Ti_{16}O_{32}$ with no dopant as a standard for reference. Observations show doping shifts the valence band and increase the slope in the conduction band with platinum having a greater effect than ruthenium. The shifts are most likely due to an increase in the number of electrons and distortions of the lattice near the dopant sites. The information can be used to show that doping titanium dioxide nanocrystals will facilitate photo induced charge transfer at the surface, which is useful in understanding photocatlytic water splitting. In the future we intend to (1) test a wide range of earth abundant elements as doping for photocatalysis and (2) explore the dynamics of photoexcited doped titania nanostructures.

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