Ab Initio Simulations of Copper Oxide Nanowires and Clusters on TiO2 (101) Anatase Surface

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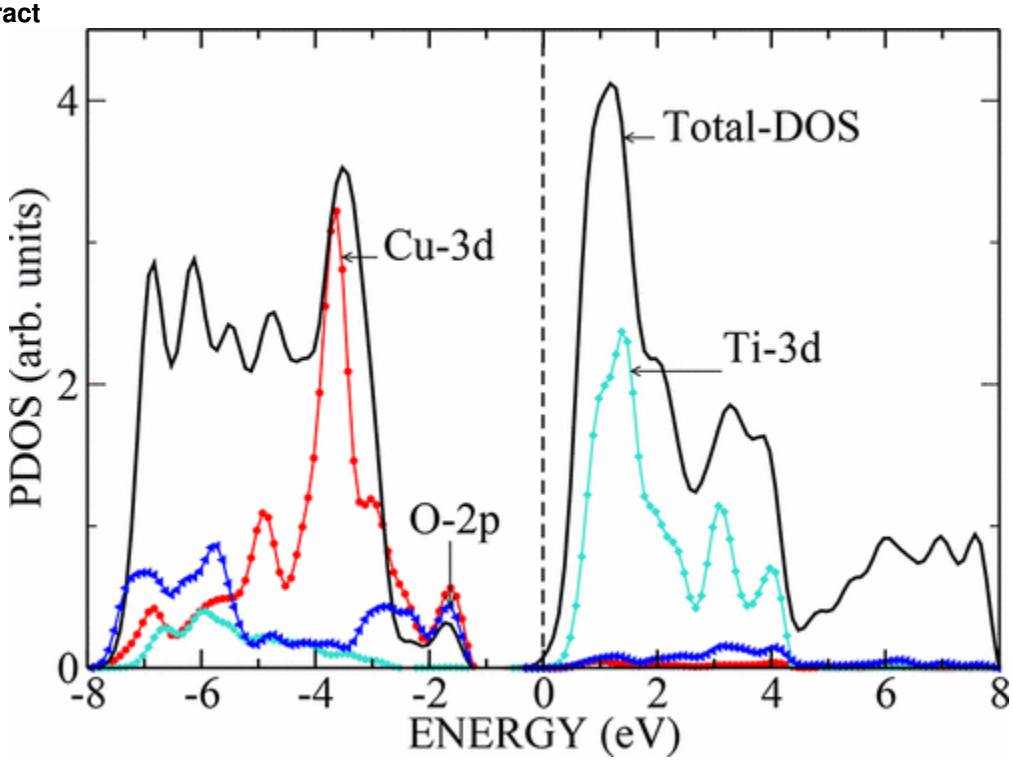
Abstract



Copper oxides deposited at titania surfaces have a beneficial effect on the photocatalytic activity of TiO_2, but their role is not fully understood. In this work, possible nanostructures of copper oxide on TiO_2 (101) have been investigated by simulations based on density functional theory. Various stoichiometries, from Cu_2O to CuO, and morphologies, from clusters to nanowires, have been considered. Nanowire structures were consistently more stable than isolated clusters. In these structures, a Cu_2O stoichiometry was found to be thermodynamically more stable than CuO at room conditions, in contrast to what happens in bulk copper. Occupied Cu 3d and O 2p states extend well into the band gap of titania, whereas the nature of the lowest-lying empty states depend on the stoichiometry: for Cu_2O

they consist mostly of Ti 3d orbitals, while in CuO unoccupied Cu 3d orbital ~0.8 eV above the Fermi level are present. Thus, both oxides reduce the band gap of the system with respect to pure titania, but only Cu_2O should be effective in separating photogenerated electrons and holes. These results provide insight into the role of copper oxides in the photocatalytic process.

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