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TÉMA

Excess Electrons in TiO2 Anatase and Rutile: Delocalized Solutions and Localized Small Polarons

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TiO2 is a prototypical metal oxide used in photocatalysis [1], photoelectrochemical (Grätzel) solar cells [2], and transparent conducting oxides [3]. Industrially two forms of TiO2 are used, rutile and anatase. The behavior of charge carriers is of key importance in virtually all applications of these materials. When excess electrons are added to the conduction band of an oxide, the electron-phonon interaction may result in electron trapping – the formation of either localized (small) or delocalized (large) polarons [4].
We used a combination of STM, STS and DFT+U to investigate the nature of electron polarons in rutile and anatase [5,6]. The excess electrons in rutile can localize at any lattice Ti atom, forming a small polaron. The polarons in rutile can easily hop to neighboring sites. Electrons in a perfect anatase lattice prefer delocalized (band-like) solutions, while electron localization is only possible at defects. Delocalized electrons were observed in Nb-doped anatase in vicinity of subsurface Nb dopants. The consequences of different electron behavior in these materials are illustrated on several examples - electrical conductivity, adsorption of simple molecules, and band alignment of rutile/anatase.

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