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Modeling electronic trap state distributions in nanocrystalline anatase¹ NAM LE, NRC Postdoctoral Associate, US Naval Research Laboratory, Washington DC 20375, IGOR SCHWEIGERT, Code 6189, US Naval Research Laboratory, Washington DC 20375 — The charge transport properties of nanocrystalline TiO₂ films, and thus the catalytic performance of devices that incorporate them, are affected strongly by the spatial and energetic distribution of localized electronic trap states. Such traps may arise from a variety of defects: Ti interstitials, O vacancies, step edges at surfaces, and grain boundaries. We have developed a procedure for applying density functional theory (DFT) and density functional tight binding (DFTB) calculations to characterize distributions of localized states arising from multiple types of defects. We have applied the procedure to investigate how the morphologies of interfaces between pairs of attached anatase nanoparticles determine the energies of trap states therein. Our results complement recent experimental findings [1] that subtle changes in the morphology of highly porous TiO₂ aerogel networks can have a dramatic effect on catalytic performance, which was attributed to changes in the distribution of trap states. [1] P. A. DeSario et al. J. Phys. Chem. C 119, 17529 (2015).

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