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Reverse-engineering the atomic-scale structure of the TiO2/N3 interface in dye-sensitized solar cells using O1s core-level shifts CHRISTOPHER PATRICK, FELICIANO GIUSTINO, Department of Materials, University of Oxford — Dye-sensitized solar cells employing mesoporous titania films sensitized with ruthenium-based dyes have shown consistently good performance over the past two decades. Understanding the process of charge injection in these devices requires accurate atomistic models of the interface between the light-absorbing dye and the semiconducting substrate. Despite considerable efforts devoted to the experimental and theoretical investigation of such interfaces, their atomistic nature remains controversial. In this work we pursue a novel computational approach to the study of the semiconductor/dye interface which does not rely on the calculated adsorption energies. In our approach we reverse-engineer photoemission data through the first-principles calculation of O1s core-level spectra for a number of candidate interface models. Our calculations allow us to discard some of the adsorption geometries previously proposed and point to an interface model which reconciles conflicting assignments based either on photoemission or infrared data.

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