

Abstract Submitted  
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**Quantitative analysis of valence photoemission spectra and quasiparticle excitations at chromophore-semiconductor interfaces**<sup>1</sup> CHRISTOPHER PATRICK, FELICIANO GIUSTINO, Department of Materials, University of Oxford, UK — Understanding electron energetics at interfaces between solids and molecules is a key challenge in many areas of nanotechnology research. Here we develop a quantitative theory of quasiparticle excitations at these interfaces and apply it to the prototypical dye-sensitized solar cell interface of N3 dye molecules adsorbed on the anatase TiO<sub>2</sub> (101) surface.<sup>2</sup> Our approach combines density-functional calculations on large interface models, bulk GW calculations,<sup>3</sup> image charge renormalization, thermal broadening and configurational disorder to obtain a quasiparticle spectrum in good agreement with experimental photoemission data. Our calculations clarify the atomistic origin of the chromophore peak at low binding energy, and illustrate the dual role played by the TiO<sub>2</sub> substrate in screening the quasiparticle states of the N3 molecule through both long-range image-charge effects and direct charge transfer via the covalently-bonded anchor groups.

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<sup>2</sup>C. E. Patrick and F. Giustino, Phys. Rev. Lett. 109, 116801 (2012)

<sup>3</sup>C. E. Patrick and F. Giustino, J. Phys. Condens. Matter 24, 202201 (2012)

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