

Abstract Submitted  
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**TiO<sub>2</sub> nanowire sensitized by natural dyes for solar cell applications**<sup>1</sup> SHENG MENG, JUN REN, EFTHIMIOS KAXIRAS, Harvard University — We investigate the electronic coupling between a semiconductor TiO<sub>2</sub> nanowire and a natural dye sensitizer based on time-dependent first-principles calculations. The model dye molecule, cyanidin is found to dissociate into the quinonoidal form upon adsorption, rendering its highest occupied molecular orbitals (HOMO) located in the middle of TiO<sub>2</sub> bandgap and its lowest-unoccupied molecular orbital (LUMO) at the bottom of TiO<sub>2</sub> conduction band. The visible light absorption is greatly enhanced with two prominent peaks at 460 nm and 650 nm. The excited electrons are injected into the TiO<sub>2</sub> conduction within a ultrafast timescale of <50 fs, with negligible non-radiative energy dissipation and recombination.

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