TiO$_2$ nanowire sensitized by natural dyes for solar cell applications$^1$ SHENG MENG, JUN REN, EFTHIMIOS KAXIRAS, Harvard University — We investigate the electronic coupling between a semiconductor TiO$_2$ 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$_2$ bandgap and its lowest-unoccupied molecular orbital (LUMO) at the bottom of TiO$_2$ 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$_2$ conduction within a ultrafast timescale of $<50$ fs, with negligible non-radiative energy dissipation and recombination.

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