Supporting Information: Improving Interfacial Charge Transfer Transitions in Nb-doped TiO₂ electrodes with 7,7,8,8-Tetracyanoquinodimethane

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Sample –	Crystallite Size [nm]	
	Anatase	Rutile
Nb 0 mol%	10.1	21.4
Nb 1.5 mol%	9.8	21.1
Nb 3.0 mol%	9.0	21.0
Nb 5.0 mol%	8.8	16.2

 $\label{eq:stable} \textbf{Table S1.} Crystallite size of TiO_2 \ samples \ with \ different \ Nb \ contents.$

Table S2. Fitting results of EIS analysis of TiO2 samples with different Nb contents.



Figure S1. (a) Reflectance spectra and optical band gaps of TiO₂ samples with different Nb contents; (b) 0, (c) 1.5, (d) 3.0 and (e) 5.0 mol%.



Figure S2. Nyquist plot of Electrochemical impedance spectroscopy (EIS) measurements based on the Undoped and Nb-doped TiO₂ Electrodes.

Figure S2 shows Nyquist plot of Electrochemical impedance spectroscopy (EIS) measurements, which were recorded under an identical forward bias of -0.40 V, which is the Voc of undoped TiO₂, was applied to all cells measured in the dark, applying a 10 mV alternating current (AC) signal over a frequency range of 10^{-1} Hz - 10^{5} Hz. From this result, Nyquist plots consist of two semicircles. The larger semicircle occurring at lower frequencies is attributed to the electron transport at the Nb-doped TiO₂-dye/electrolyte interface. Fitting the lower frequency semicircle subsequently gives capacitance(C μ) and resistance (R_{rec}). Indeed, Comparing Nb doped TiO₂ (1.5 mol%) with undoped one, C μ decreased from 2606 to 2568 μ F cm⁻², while R_{rec} increased from 37.7 to 47.7 Ω (Table S2). From the lower C μ , a negative band edge sift was induced and electron-back-contact from Nb doped TiO₂ interface to TCNQ dye was found by increasing R_{rec}. Therefore, passivation at the surface was implied by electronic physics analytics in the device containing the Nb-doped TiO₂ (1.5 mol%) electrode.



Figure S3. Conversion efficiency of DSSCs employing different Nb dopants, and the values are mean and standard deviation (error bars) of 3 replicates for each device.