

Supporting Information

Niobium-doped (001) Dominated Anatase TiO₂ Nanosheets as Photoelectrode for Efficient Dye-Sensitized Solar Cells

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Table S1. Calculated bond length between bonded surface Ti atom of the TiO₂ surface and dye O atom in the carboxylic group. (unit in Å)

	Bond I	Bond II	Bond III
N719+(101)	1.922	2.017	1.954
N719+(101)-Nb-T	1.892	1.984	1.925
N719+(101)-Nb-B	1.904	1.990	1.937
N719+(100)	1.958	1.972	2.314/2.051
N719+(100)-Nb-T	1.940	1.953	2.309/2.033
N719+(100)-Nb-B	1.949	1.963	2.329/2.038
N719+(001)	1.973	2.079	2.080/2.206
N719+(001)-Nb-T	1.962	1.984	2.091/2.140
N719+(001)-Nb-B	1.964	1.984	2.069/2.145

Table S2. Surface properties of different TiO₂ surface – N719 dye systems.

Surface	Experiment			Calculation
	BET	M _{Ru}	N _A	N _A
	(m ² /g)	(mg/g)	(molecule/nm ²)	(molecule/nm ²)
(101)	62.1	3.86	0.39	0.24
(100)	53.5	3.82	0.45	0.28
(001)	88.1	5.13	0.37	0.28
Nb-(101)	147.8	8.23	0.37	0.24
Nb-(100)	85.5	4.36	0.32	0.28
Nb-(001)	91.0	6.79	0.48	0.28

Table S3. Calculation: the percentage of active facets on TiO₂ nanosheets = $2(\text{length} \times \text{width}) / (2(\text{length} \times \text{width}) + 2(\text{length} \times \text{thickness}) + 2(\text{width} \times \text{thickness}))$.

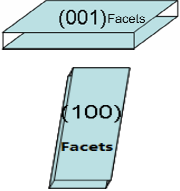
	Average length (nm)	Average width (nm)	Average Thickness (nm)	Percentage
(001)-TiO ₂ -NS	~47	~47	~5	~82.5%
Nb-(001)-TiO ₂ -NS	~50	~50	~5	~83.3%
(100)-TiO ₂ -NS	~110	~30	~4	~85.5%
Nb-(100)-TiO ₂ -NS	~150	~35	~4	~87.6%

Table S4. Nb content in the TiO₂ nanosheets determined using ICP-OES, EDS measurement and the theoretical doping amount.

samples	Measurement		Theoretical Doping (mol%)
	(mol%) ICP	(mol%) EDS	
Nb-doped-(101)-TiO ₂ nanoparticles	2.51	3.0	2.50
Nb-doped-(100)-TiO ₂ nanosheets	2.10	1.7	2.00
Nb-doped-(001)-TiO ₂ nanosheets	2.52	2.2	2.00

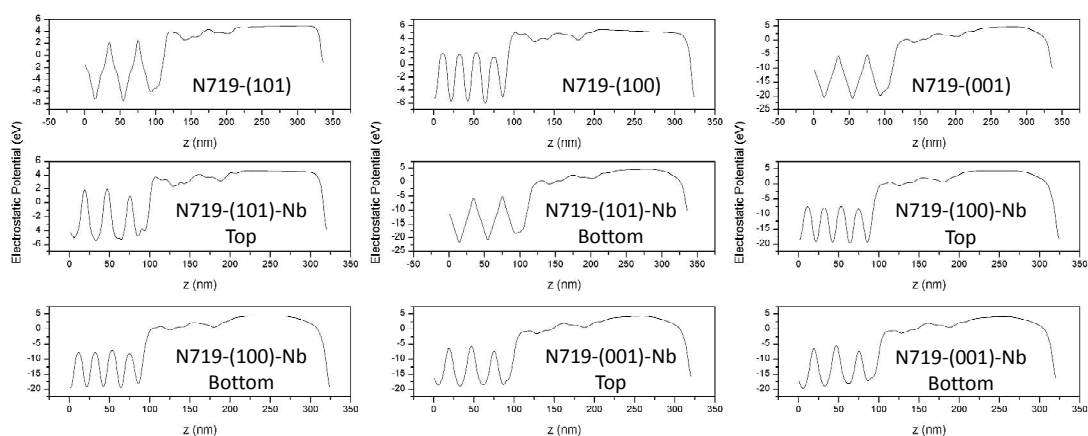


Figure S1 Work function (WF) of different TiO_2 surface – N719 dye combined systems.

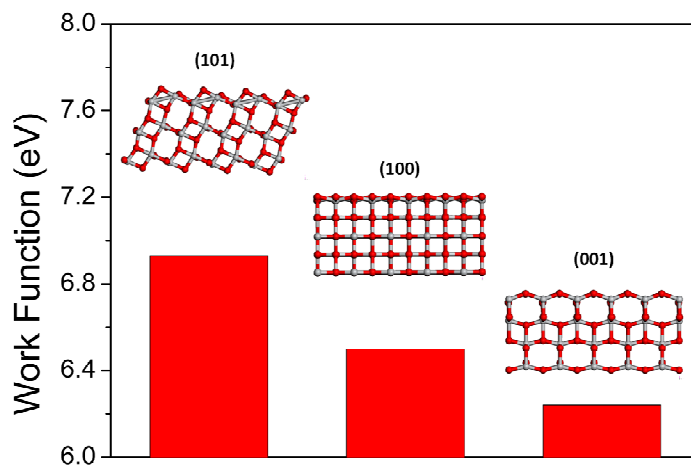


Figure S2. (101), (100) and (001) anatase surfaces with the work function level from DFT calculations.

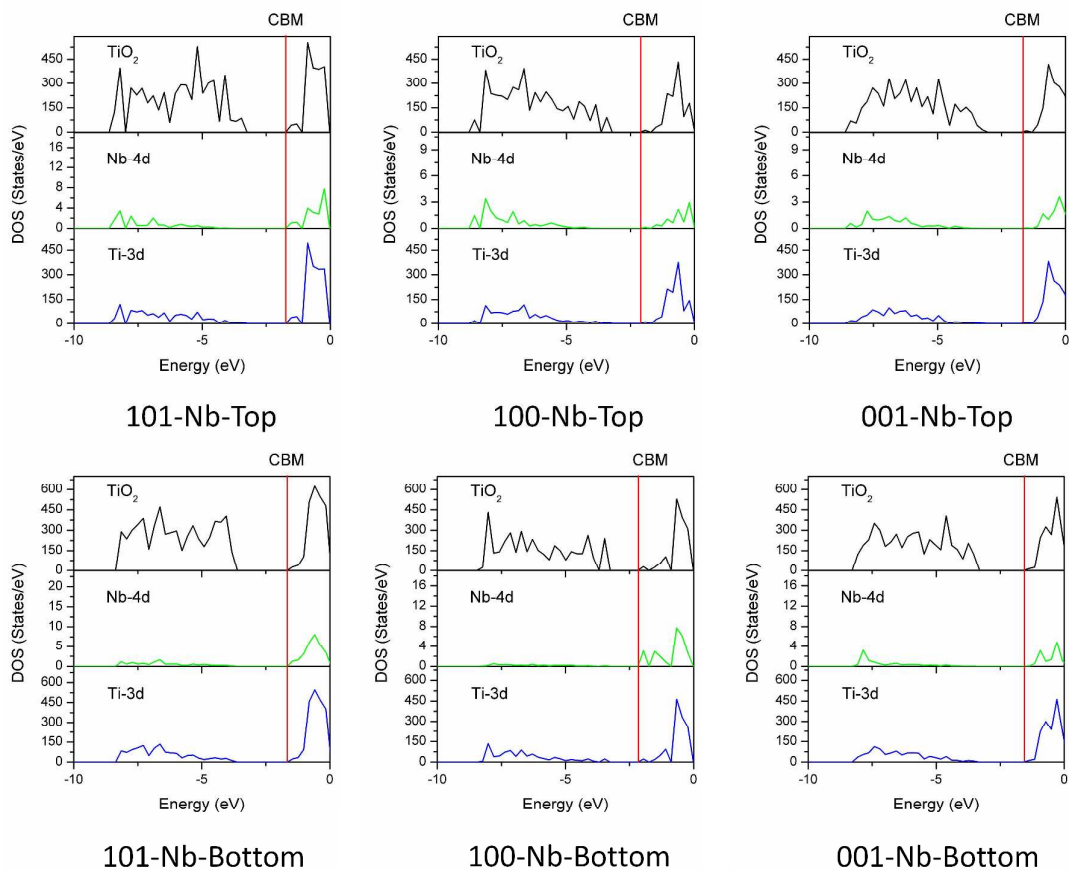


Figure S3. The density of states (DOS) of Nb-doped anatase TiO_2 and its partial DOS of Ti $3d$ and Nb $4d$.

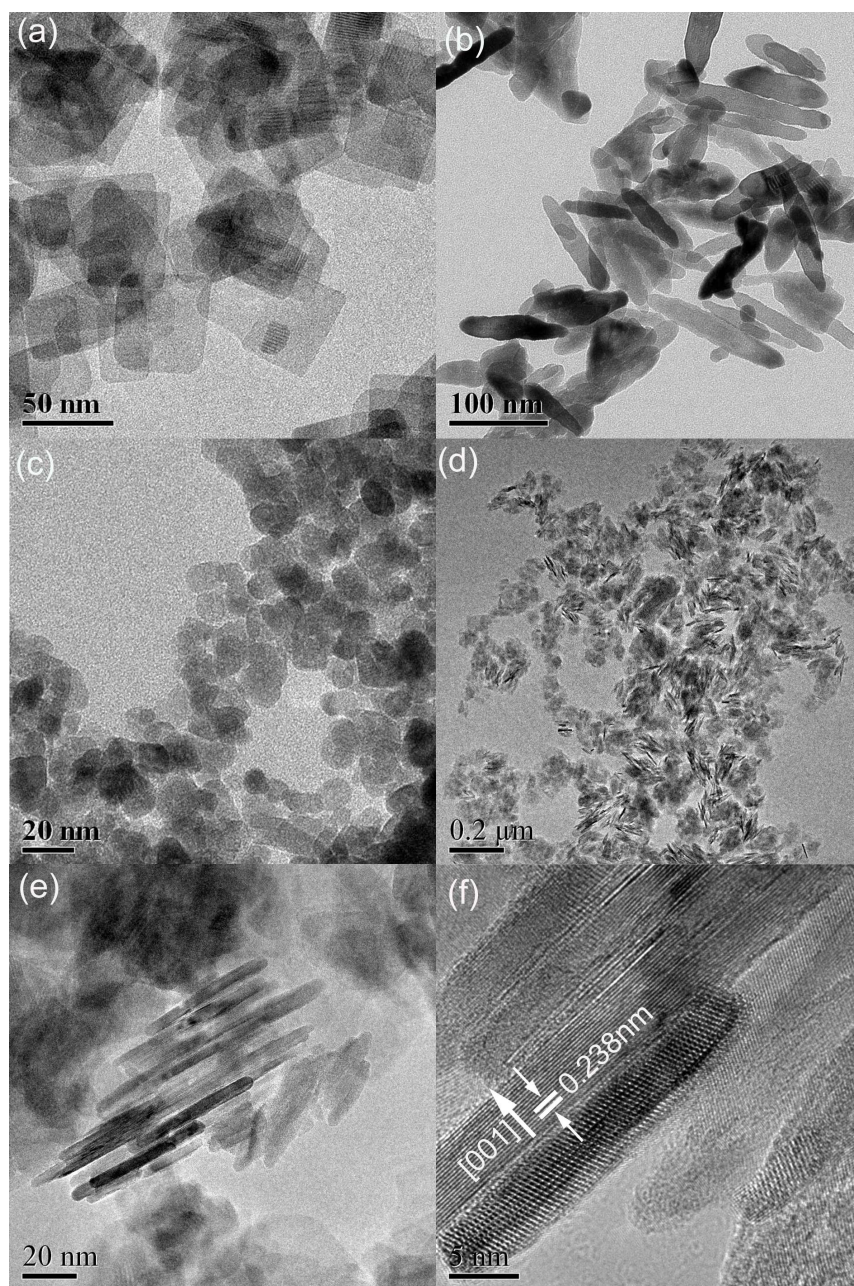


Figure S4 (a) TEM image of (001) nanosheets. (b) TEM image of (100) nanosheets. (c) TEM image of Nb-doped (101) nanoparticles. HRTEM of Nb-doped (001)-oriented TiO_2 nanosheets, (d), (e) and (f).

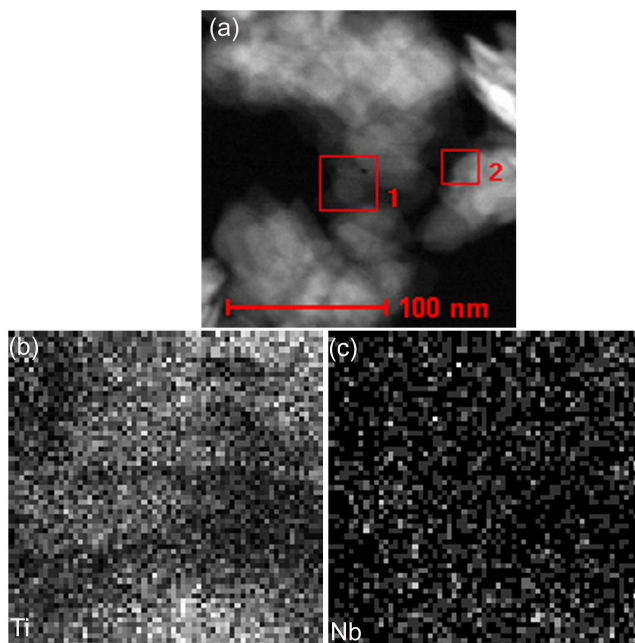


Figure S5 (a) Dark-field STEM image of Nb-doped (001) TiO₂ nanosheets. (b) The corresponding elemental mapping of Ti atoms. (c) The corresponding elemental mapping of Nb atoms.

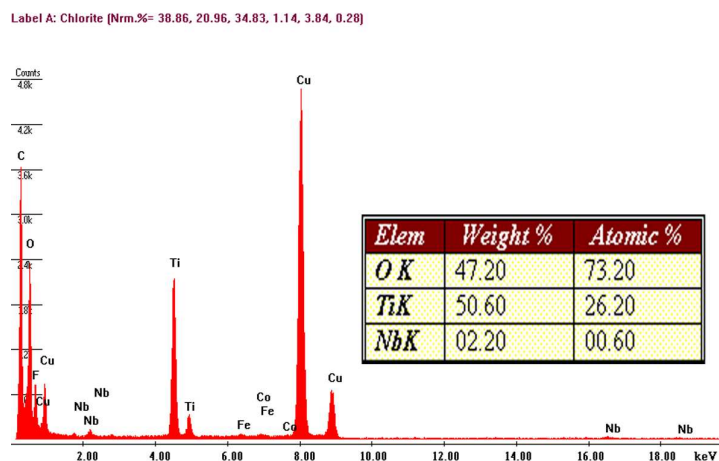


Figure S6 The EDS image of Nb-doped (001)-oriented TiO₂ nanosheets.

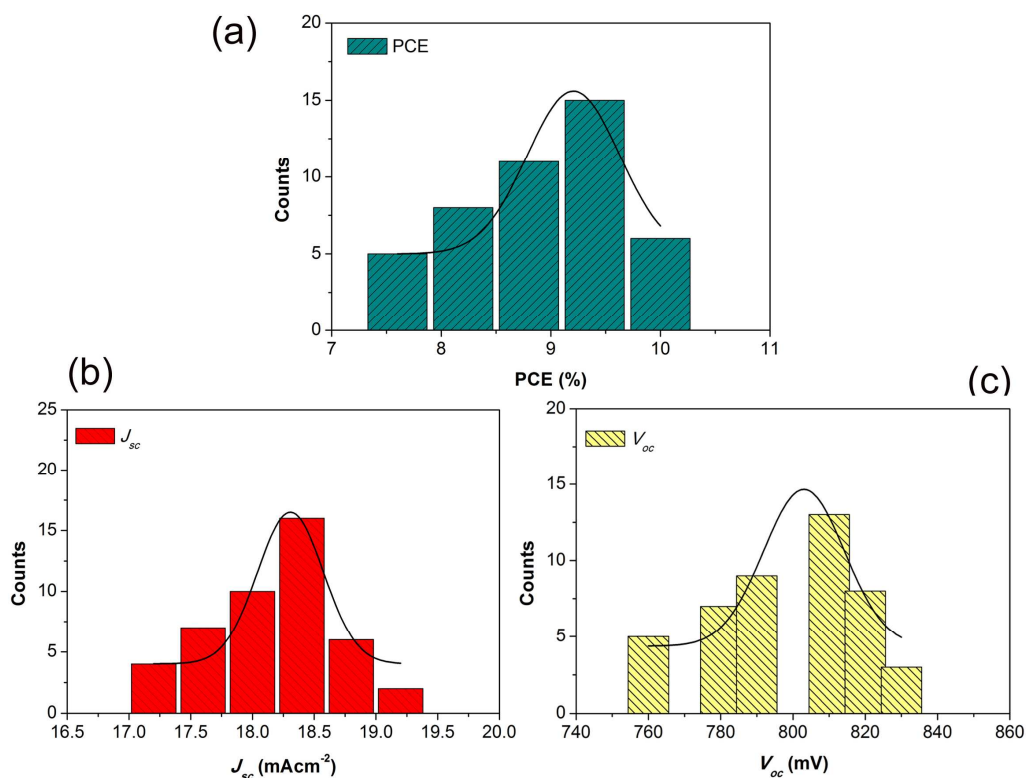


Figure S7 (a) Histogram plots of solar photo-conversion efficiency (PCE) for a large batch of devices (total of 45 devices) based on Nb-doped (001) TiO_2 nanosheets electrodes. The total of DSSCs based on Nb-doped (001) TiO_2 nanosheets have been made 45 devices, and the photo-conversion efficiency (η) more than 9% have 21 devices. (b), (c) distribution histogram of the open-circuit photovoltage and short-circuit photocurrent density.

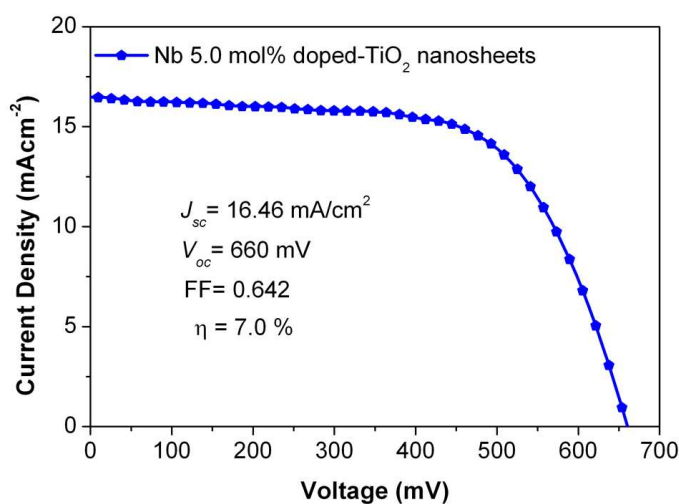


Figure S8 J - V curves of dye-sensitized solar cells based on Nb 5.0 mol% doped (001)- TiO_2 electrodes.