Supporting Information

Origin of efficiency enhancement in Nb_2O_5 coated titanium dioxide nanorod based dye sensitized solar cells.

Eva Barea,[a*] **Xueqing Xu,**[a,b] **Victoria González-Pedro,**[a] **Teresa Ripollés-Sanchis,**[a] **Francisco Fabregat-Santiago**[a*] **and Juan Bisquert**[a]

[a] Grup de Dispositius Fotovoltaics i Optoelectrònics, Departament de Física. Universitat Jaume I, 12071, Castelló, Spain

[b] Guangzhou Institute of Energy Conversion, Renewable Energy and Gas Hydrate Key Laboratory of Chinese Academy of Sciences, Guangzhou 510640, China

Corresponding authors email: fran.fabregat@fca.uji.es, barea@fca.uji.es

Contribution to the special number of the International Conference on Ordered 1 Dimensional Nanostructures for Photovoltaics, from 12 to 15 september 2010, Mallorca, Spain

Recombination resistance and Chemical capacitance vs potential:

For most of the cases, the charge transfer resistance arising at the porous nanostructured electrode in contact with liquid electrolyte may be described by using a recombination resistance (or charge transfer resistance), R_{rec}, that depends on the Fermi level as:[1, 2]

$$R_{rec} = R_0 \exp\left[\beta \frac{E_{redox} - E_{Fn}}{k_B T}\right] \tag{S1}$$

in which R_0 is a constant indicating the onset of recombination, β is the recombination parameter (also named charge transfer coefficient) governing the non linear recombination, k_B is the Boltzmann constant, T the temperature, E_{Fn} the Fermi level of electrons in the semiconductor and E_{redox} the redox potential (i.e. the Fermi level of holes in the electrolyte). The Fermi level voltage is $V_F = (E_{Fn} - E_{redox})/q$, with q the electron charge, and thus Eq. (S1) may be written as Eq. (1).

The capacitance of these nanostructures, when they have a low doping, is described by the equation: [3]

$$C_\mu = \frac{N_c q^2}{k_B T} \exp\left[\frac{E_{Fn} - E_C}{k_B T_0}\right] \tag{S2}$$

C_μ is known as chemical capacitance and describes the density of states (DOS) of the nanostructured photoanode at energy levels below the conduction band (E_c) given by the tail of the Boltzmann distribution. For a given number of states below the conduction band, N_c, this DOS is determined by the tail parameter T_0, which has units of temperature, and by the position of the conduction band. Eq. (S3) is usually written in terms of $\alpha = T/T_0$ and of V_F, yielding:

$$C_\mu = C_0 \exp\left[\alpha \frac{qV_F}{k_B T}\right] \tag{S3}$$

Effects of recombination resistance and photocurrent in *j-V* curves

Eqs. (6) and (7) generate the *j-V* curves shown in Fig. S1. The larger R_0 (smaller j_0), produces a larger R_{rec} as plot in Fig. S1(a) and, for the same j_{sc}, a larger V_{oc} as may be seen in Fig. S1(b). For the same R_0, an increase in j_{sc} produces a larger V_{oc}, as shown in Fig. S1(c).

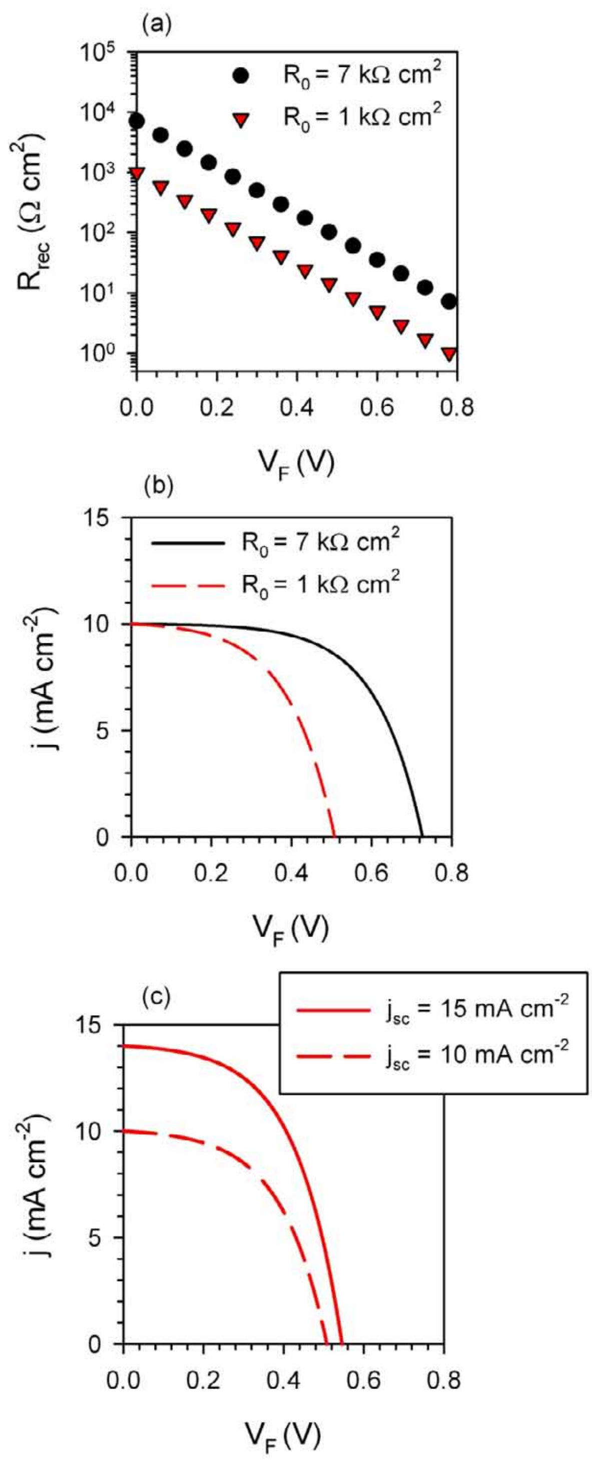

Fig. S1: (a) Simulation of recombination resistance with $\beta = 0.23$, $R_0 = 7$ kΩ cm^{-2} (circles) and $R_0 = 1$ kΩ cm^{-2} (triangles). (b) *j-V* curves simulated from the simulated resistances in (a) with $j_{sc} = 10$ mA cm^{-2}. (c) *j-V* curves simulated from the simulated resistance with $R_0 = 1$ kΩ cm^{-2}, $j_{sc} = 15$ mA cm^{-2} (solid line) and $j_{sc} = 10$ mA cm^{-2} (dashed line).

References

1. F. Fabregat-Santiago, J. Bisquert, E. Palomares, L. Otero, D. Kuang, S. M. Zakeeruddin and M. Grätzel, *The Journal of Physical Chemistry C*, 2007, 111, 6550-6560.
2. Q. Wang, S. Ito, M. Grätzel, F. Fabregat-Santiago, I. Mora-Seró, J. Bisquert, T. Bessho and H. Imai, *The Journal of Physical Chemistry B*, 2006, 110, 19406-19411.
3. J. Bisquert, *Phys. Chem. Chem. Phys.*, 2003, 5, 5360.