Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Stability of Dye-Sensitized Solar Cells under Extended Thermal Stress

*Surendra K. Yadav[1], Sandheep Ravishankar[2], Sara Pescetelli[1], Antonio Agresti[1], Francisco Fabregat-Santiago[2], Aldo Di Carlo[1]**

[1]C.H.O.S.E. (Centre for Hybrid and Organic Solar Energy), Department of Electronic Engineering, University of Rome "Tor Vergata", via del Politecnico 1, Rome, 00133 Italy.

[2]Group of Advanced Materials and Energy, Institute of Advanced Materials, Universitat Jaume I, Castello de la Plana, Avda. V. Sos Baynat s/n, 12006, Spain

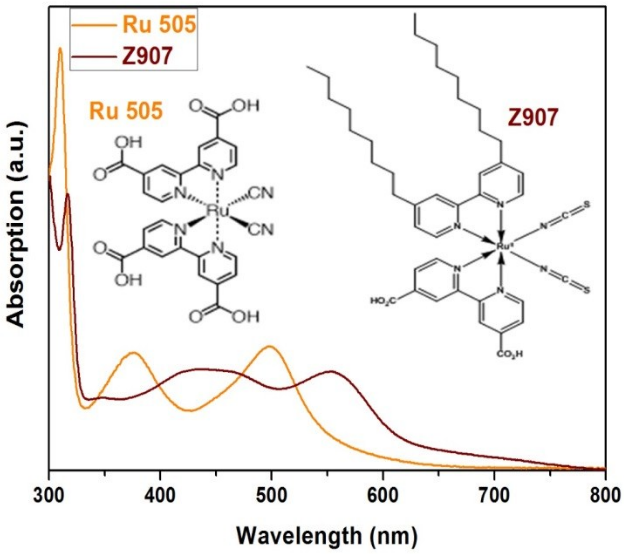

Fig. S1: Chemical structure of employed dye Z907 and Ru505 differing mainly in the ancillary ligand attached to the central metal atom, such as SCN and CN respectively. The absorption onset extends towards higher wavelength in Z907 when compared with Ru505.

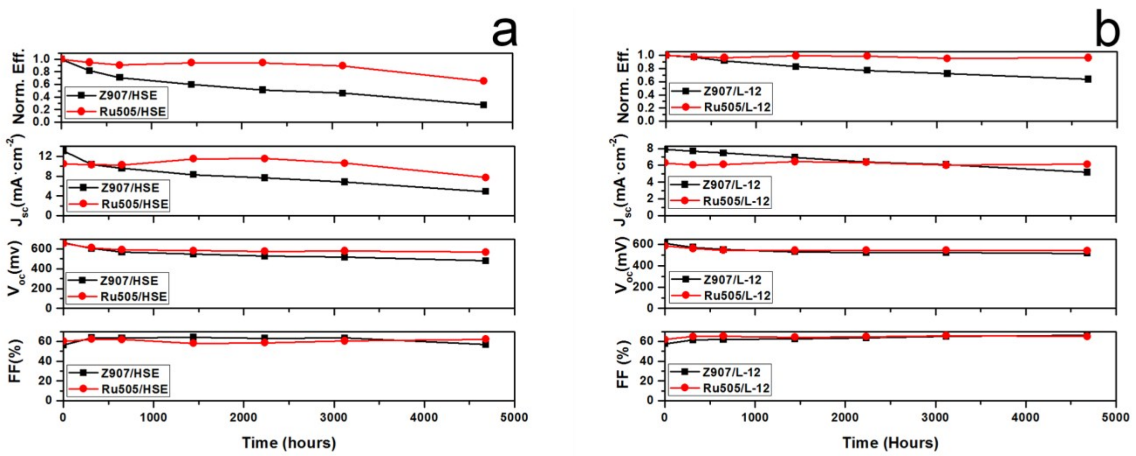

Fig. S2: The electrical parameters for a) Z907/HSE and Ru505/HSE b) Z907/L-12 and Ru505/L-12, under temperature stress at 85°C as a function of time under 1 sun AM 1.5G 1000 W/m^2.

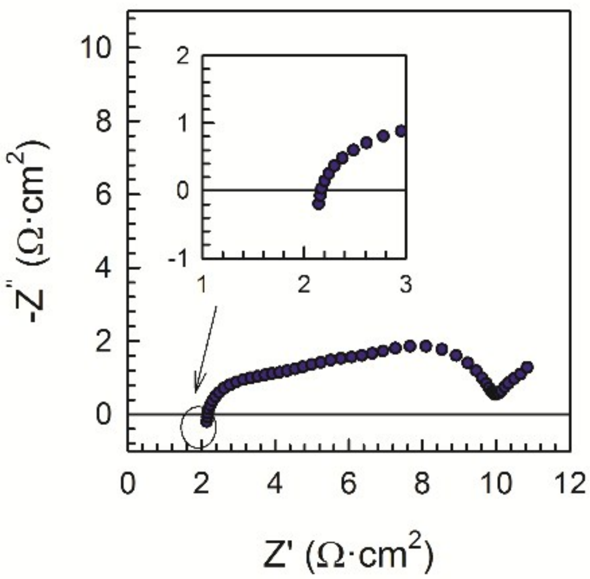

Fig. S3: Nyquist spectra of Z907/L-12 samples at -0.62 V showing the inductive effect at high frequencies.

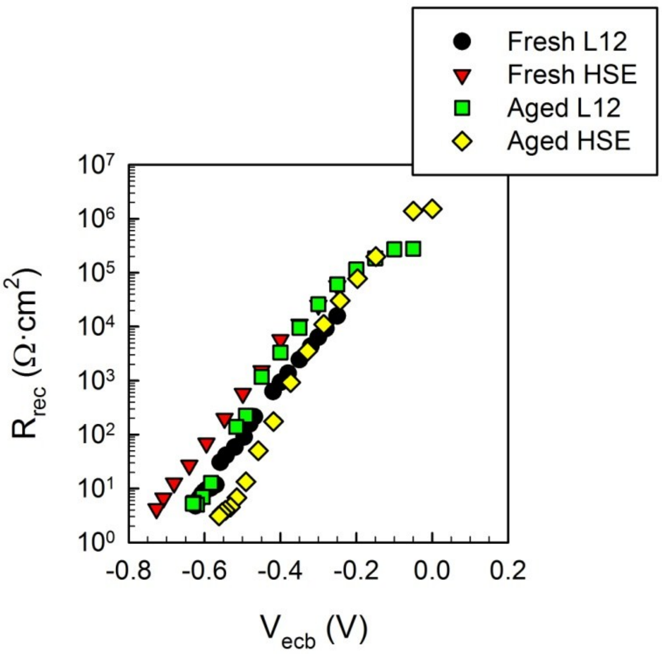

Fig. S4: Plot of recombination resistances versus voltage at equivalent conduction band for Z907 samples

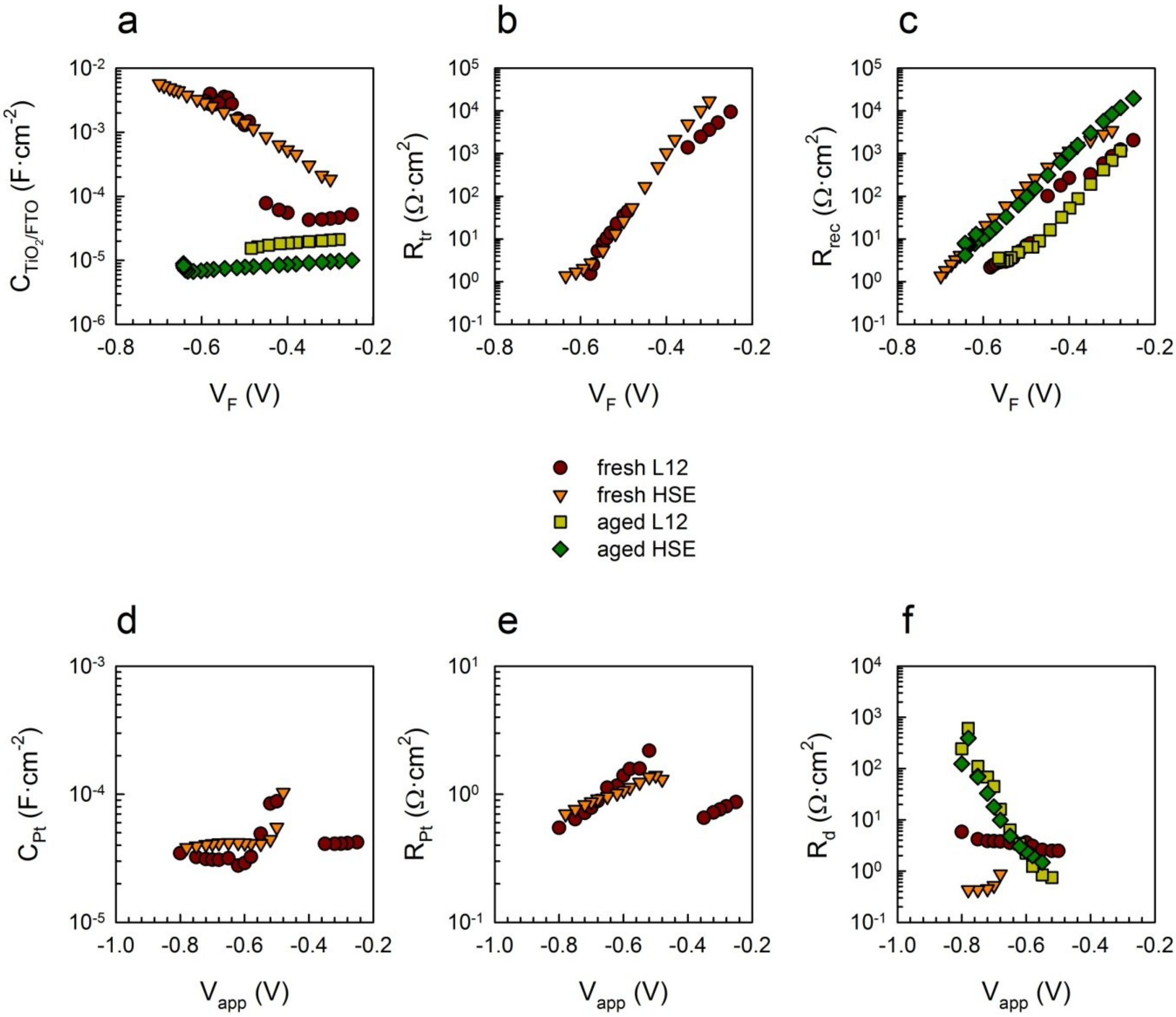

Fig. S5: a) Conduction band capacitance b) Recombination resistance c) Transport resistance d), e) Pt counter electrode capacitance and resistance respectively f) Ionic diffusion resistance and g) Capacitance of the FTO, for fresh and aged Ru505-based devices.

From the recombination resistances (Fig. S5b), it can be seen that sample aging does not affect the recombination properties of the cell in a very significant way. Only a slight shift (few mV) towards lower voltage is found in HSE aged sample with respect to fresh one.

However, the recombination in the L-12 samples is displaced ~ 200mV towards lower potentials as compared to the HSE samples, so the V_{oc} is expected to be higher in HSE cells as compared to L-12 cells.

Moreover, in the case of aged Ru505 samples, the transmission line could not observed for both employed electrolytes. This suggests TiO_2/electrolyte interface modifications, already observed in literature as a consequence of concurrent phenomena, such as formation of a solid electrolyte interphase (SEI) layer wrapping TiO_2 surface and/or aging induced shift of TiO_2 conduction band leading to a V_{OC} reduction, as observed in Fig. 2b reported in the main text.

The evolution of the counter electrode capacitance and charge transfer resistance (Fig. S5d and e) is consistent with that obtained from the Z907 case.

The diffusion resistance (Fig. S5f) increases exponentially for aged HSE sample, indicating that the electrolyte is losing its transport properties, mainly due to electrolyte bleaching and/or leakage and eventually leading to the performance loss. The diffusion resistance is higher for L-12 cells as compared to HSE cells, which is in accordance with the nature of the respective electrolytes as observed from IS measurements on Z907 cells, see Fig. 6f in the main paper.

The capacitance of the FTO remains stable under thermal stress for the L-12 samples but is reduced by an order of magnitude for the HSE samples. This suggests that the FTO is either losing contact with electrolyte testifying its leakage.