

Effects of Plasmonic Nanoparticle Incorporation on Electrodynamics and Photovoltaic Performance of Dye Sensitized Solar Cells

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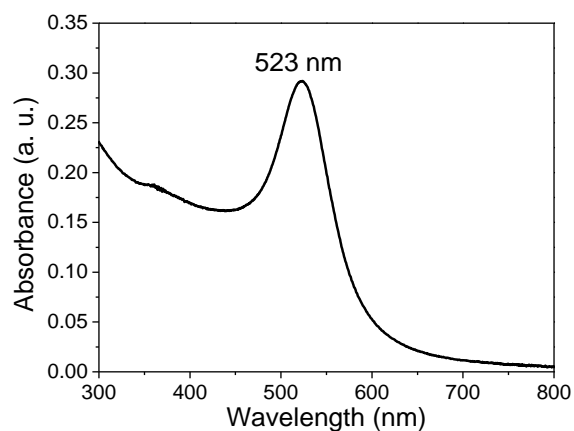


Figure S1. Absorption spectrum of the as-synthesized gold colloid.

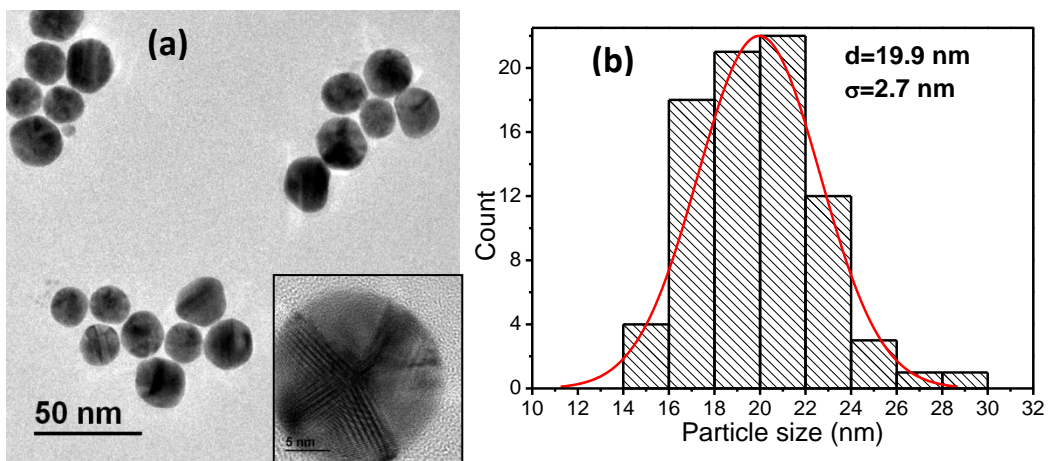


Figure S2. (a) Typical TEM micrograph of the gold nanoparticles. Inset shows the HRTEM micrograph of a representative Au nanoparticle, revealing its crystallinity and structural defects. (b) The size distribution histogram of Au nanoparticles and its Gaussian fit, revealing 19.9 nm average size and 13 % of size dispersion.

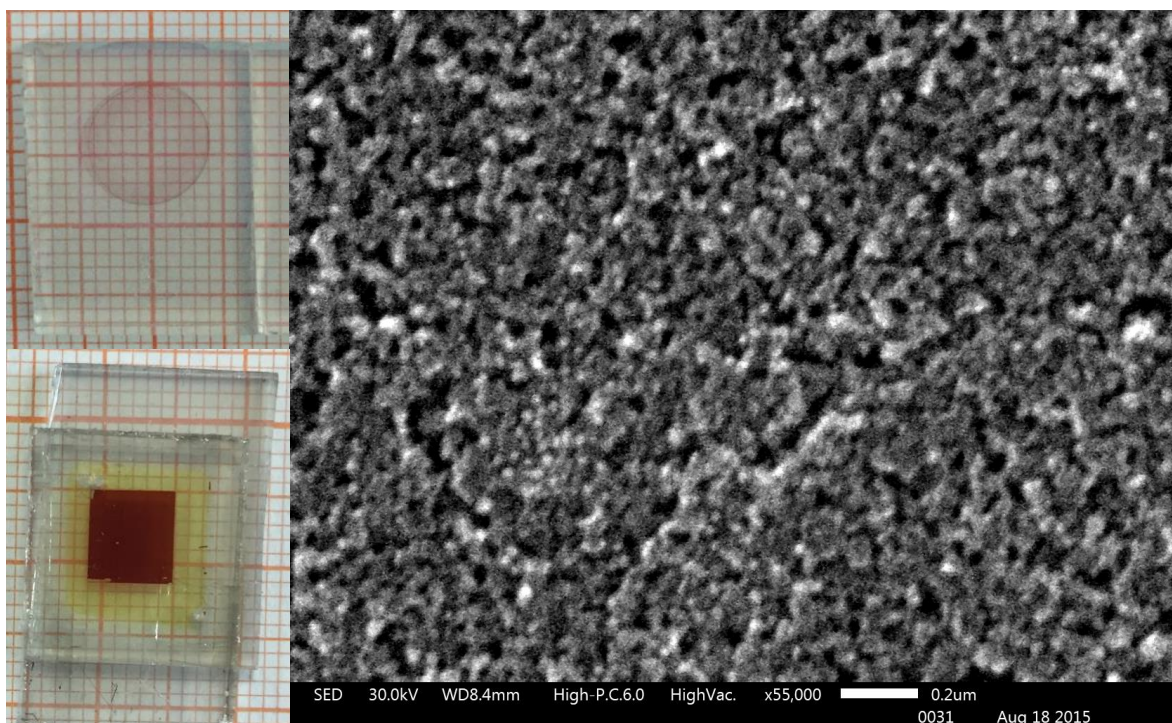


Figure S3. SEM image of the TiO_2 film with 5 Au NP treatments after firing at 350°C .

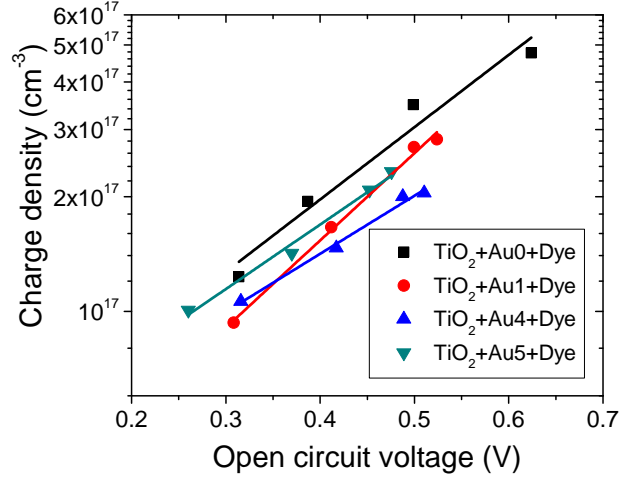


Figure S4. Electron charge density vs open circuit voltage plots as a function of light intensity for samples with different Au NP treatments.

The trap distribution parameter α' was obtained by fitting the slope of the open circuit voltage (V_{OC}) vs electron charge density (n) plots using the relation:¹

$$n = n_0 \exp[\alpha' eV / (k_B T)] \quad (s1)$$

where k_B is the Boltzmann constant, e is the absolute value of electron charge, T is the cell temperature (25 °C), and V is the cell voltage. The electron charge density in dark n_0 is obtained by extrapolation of charge density to $V_{OC}=0$. (dark condition).

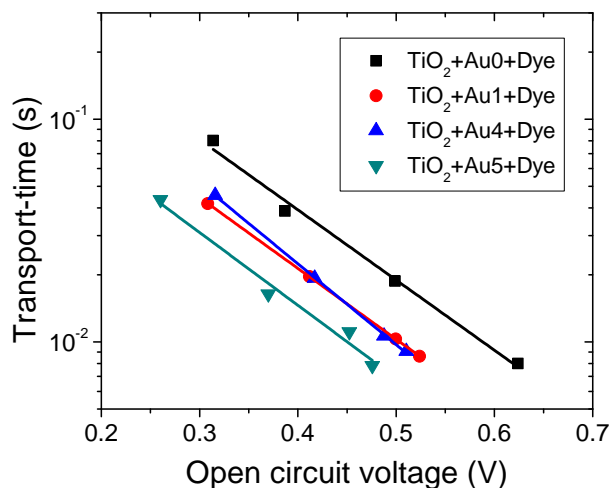


Figure S5. Electron transport-time vs open circuit voltage plots as a function of light intensity for samples with different Au NP treatments.

The non-ideality factor of free electron parameter^{2,3} b was obtained by fitting the slope of the electron transport-time τ_{tr} (as obtained from SLIT of photovoltage measurements) vs open circuit voltage plot using the relation:¹

$$\tau_{tr} = \tau_{tr,0} \exp \left[-\frac{(1-\alpha'b)eV}{\alpha'b(k_{\beta}T)} \right] \quad (s2)$$

and the previously determined α' (Fig. S4).

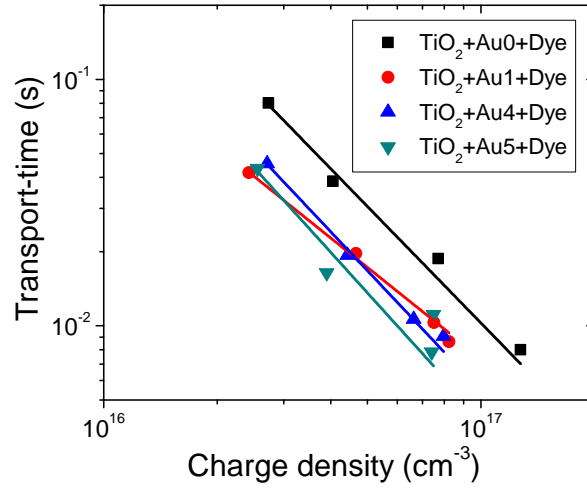


Figure S6. Electron transport-time vs charge density plots as a function of light intensity for samples with different Au NP treatments.

The transport-time in dark $\tau_{tr,0}$ was obtained by fitting the electron transport-time τ_{tr} vs charge density plots using the relation:¹

$$\tau_{tr} = \tau_{tr,0} \left[\frac{n}{n_0} \right]^{-\frac{1-\alpha'b}{\alpha'b}} \quad (\text{s3}),$$

and the previously estimated α' and b values (Figs. S4 & S5) and extrapolating the fitted curves to $n=n_0$ (dark conditions) for each DSSCs with different Au NP treatments obtained from Figure S4. The diffusion coefficient in dark D_0 was obtained utilizing the relation:⁴

$$D_0 = \frac{a^2}{2.77\tau_{tr,0}} \quad (\text{s4}).$$

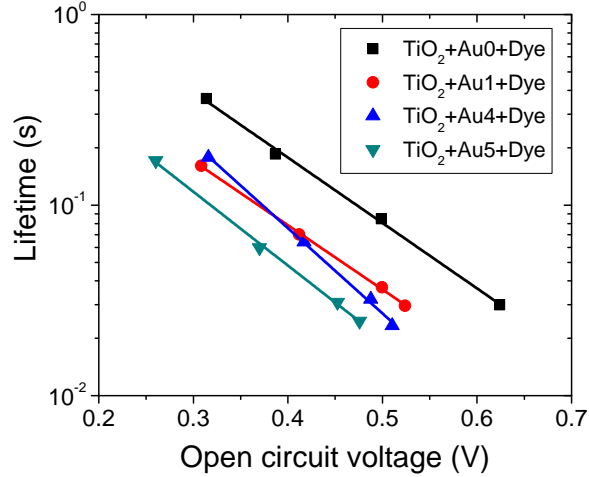


Figure S7. Electron lifetime vs open circuit voltage plots as a function of light intensity for samples with different Au NP treatments.

The nonlinear recombination parameter β was obtained by fitting the slope of the electron lifetime τ_r vs open circuit voltage plots using the relations:¹

$$\tau_r = \tau_{r,0} \exp \left[-\frac{(\beta - \alpha'b)eV}{\alpha'b(k_B T)} \right] \quad (s5)$$

and the previously estimated α' and b values. The electron lifetime in dark $\tau_{r,0}$ was obtained by extrapolating the fitting curves to $V_{OC}=0$ (dark conditions) for each DSSCs with different Au NP treatments.

The as-obtained parameters are summarized on Table S1. These parameters were used to calculate the J-V curves with the aid of total electron density model (eq. 2 of the main text), assuming a total series resistance R_s (Used to fit the experimental maximum power generated by the DSSCs). Figure S8 compares the calculated J-V curves with the corresponding experimental ones measured for DSSCs with different Au NP treatments. In Equation 2 of the main text the trap distribution parameter is defined as $\alpha = \alpha'b$.

Table S1. Fitting parameters obtained from SLIT of photovoltage and photocurrent measurements for the different Au treated DSSCs.

Parameter	Au0	Au1	Au4	Au5
α'	0.114	0.137	0.091	0.101
β	1.0	1.0	1.0	1.0
b	3.308	3.053	3.242	3.367
n_0 (m ⁻³)	2.83 x10 ¹⁶	1.84 x10 ¹⁶	2.19 x10 ¹⁶	3.08 x10 ¹⁶
D_0 (m ² s ⁻¹)	5.18x10 ⁻¹¹	6.00 x10 ⁻¹¹	6.60 x10 ⁻¹¹	1.25 x10 ⁻¹⁰
k_0 (s ⁻¹) fit	0.818	0.650	1.523	0.960
η_{inj} fit	0.596	0.498	0.472	0.426
d (μm)	3.6	3.6	3.6	3.6
R_s (Ω)	17.84	20.25	19.57	14.64

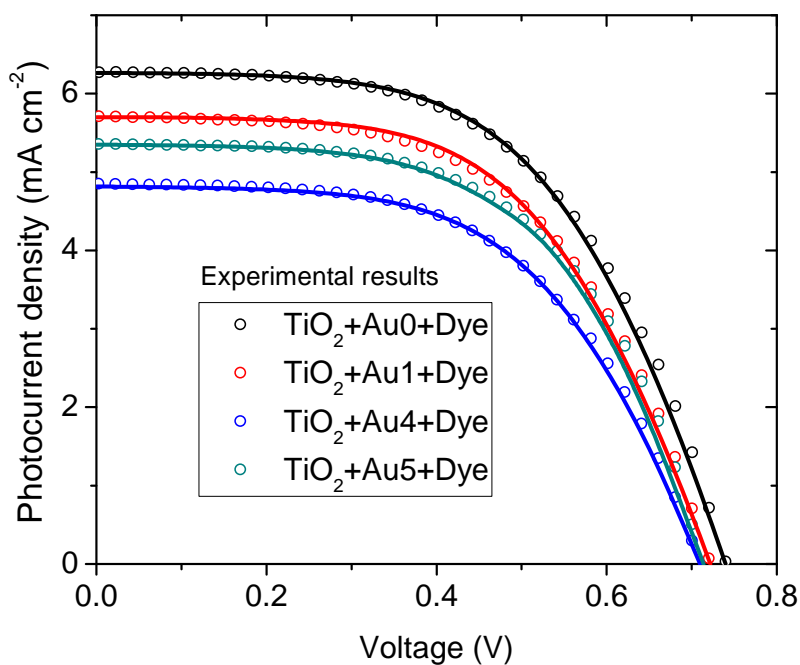


Figure S8. Comparison between the measured (symbols) and theoretical (continuous) current vs voltage curves for the DSSCs prepared with different Au NP treatments.

References

1. Anta, J. A. et al. A Continuity Equation for the Simulation of the Current–Voltage Curve and the Time-Dependent Properties of Dye-Sensitized Solar Cells. *Phys. Chem. Chem. Phys.* **2012**, *14*, 10285-10299.
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