Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information

Efficiency enhancement in dye-sensitized solar cells using shape-dependent plasmonic nanocomposite photoanodes incorporating silver nanoplates

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1. 3D modeling for finite element analysis

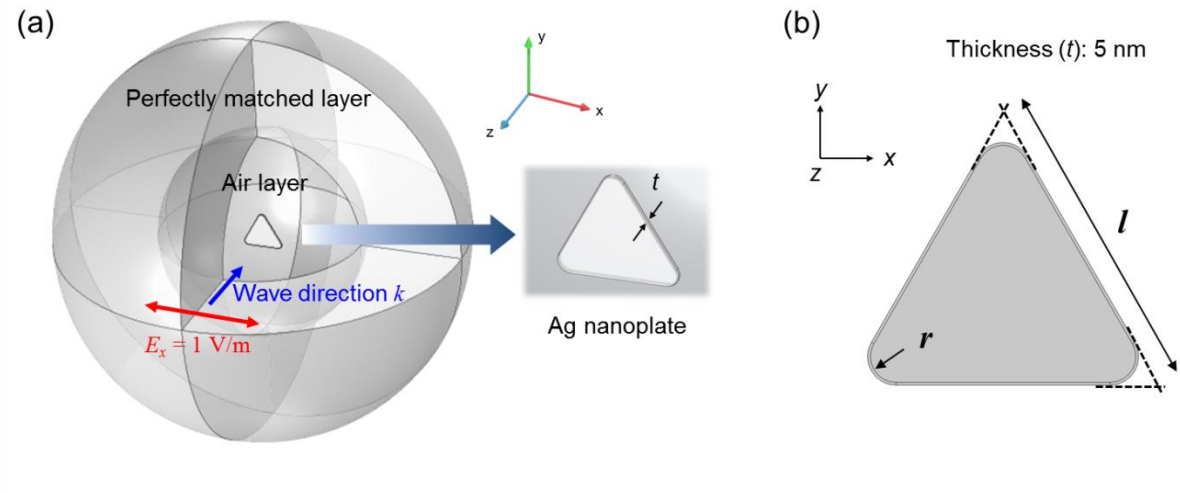

Figure S1. (a) 3D numerical model used for FEM analysis and (b) schematic illustration of Ag nanoplate.

A single Ag nanoplate was placed on a center surrounded by air layer. Also, perfectly matched layer (PML) was additionally modeled on air layer for prevention of backscatter from these boundaries. Radii of air layer and PML were λ/2 and λ respectively, where λ is the incident wavelength of light. The nanoplate was set as an equilateral triangle with the side length (*l*) from 60 nm to 180 nm, maintaining the thickness of 5 nm. Radius of curvature (*r*) at three nanoplate corners was varied from 10 nm to 26 nm to investigate shape effect on the plasmon resonance wavelength (figure S1(b)). The

minimum mesh size was 3 nm around the nanoplate, and the maximum size of air layer was one fifth of the wavelength.

By assuming time-harmonic electrid field, this model solves the electric field $\vec{E}(r,t)$ using Maxwell's equation (1) [30]:

$$\nabla \times \mu_r^{-1}(\nabla \times \vec{E})k_0^2 - \left(\varepsilon_r - \frac{j\sigma}{\omega\varepsilon_0}\right)\vec{E} = 0 \quad (1)$$

where the constants μ_r and ε_r are relative permeability and complex value of relative permittivity, respectively. The material property of Ag were obtained from Ref. [31]. The electric field (i.e. incident light) was propagated through z-direction with peak amplitude of E_x = 1 V/m (see figure S1a). Using a parametric sweep analysis, wavelength λ was varied from 350 nm to 1100 nm. To calculate scattering energy, we used a well-known scattered field formula which is calculated by integrating Poynting vector of the scattered field over the surface of nanoplate.

2. Spectrum of solar radiation

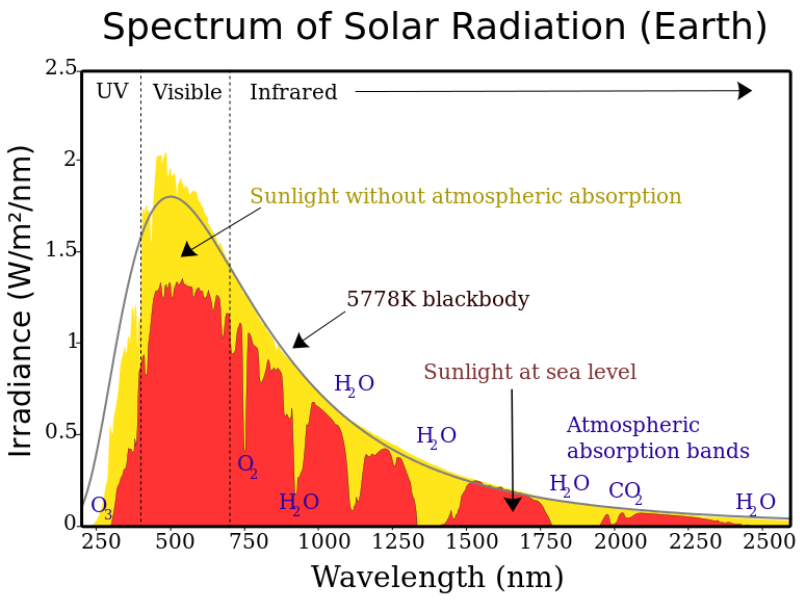

Figure S2. Solar irradiance spectrum above atmosphere and at surface. Extreme UV and X-rays are produced (at left of wavelength range shown) but comprise very small amounts of the Sun's total output power. (reference: Iqbal, M., "An Introduction to Solar Radiation", Academic Press (1983), Chap. 3)

3. Transient heat transfer analysis

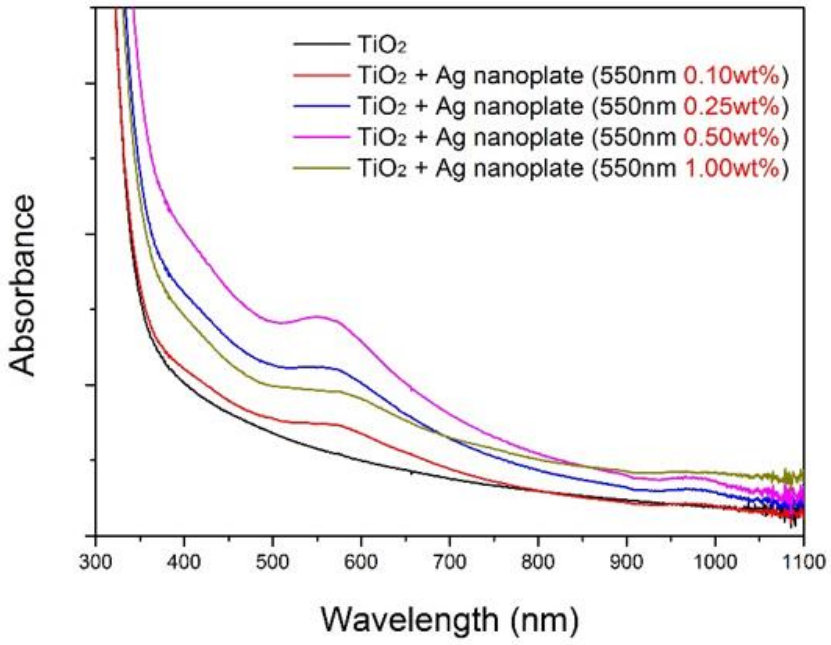

Figure S3. UV-vis absorbance spectra of the Ag nanoplate-incorporated plasmonic photoanodes with different weight fraction of Ag nanoplates.