SUPPORTING INFORMATION

Dielectric Band Edge Enhancement of Energy Conversion
Efficiency in Photonic Crystal Dye-Sensitized Solar Cell

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Simulation Methodology

This supporting information file contains the simulation methodology for electromagnetic wave propagation through a TiO_2 inverse opal and a TiO_2 nanocrystalline film bilayer. Simulations were performed with the finite-difference time-domain (FDTD) method ¹, using a freely available software package (MEEP) with subpixel smoothing for increased accuracy ². MEEP is a free finite-difference time-domain (FDTD) simulation software package developed at Massachusetts Institute of Technology to model electromagnetic systems.

MEEP FDTD simulation and parameters

Diameter ($2r$) of sphere: 285nm.

Direction of axes: following MEEP convention.

Location of spheres: FCC structure with (111) on y-z plane.

(x,y,z)

($-r\sqrt{3}$, r , 0)

($-r\sqrt{3}$, $-r$, 0)

(0, $2r$, 0)

(0, 0, 0)

(0, $-2r$, 0)

($r\sqrt{3}$, r , 0)

($r\sqrt{3}$, $-r$, 0)

($-r\sqrt{3}$, $2r$, $r\sqrt{3}$)

($-r\sqrt{3}$, 0, $r\sqrt{3}$)

($-r\sqrt{3}$, $-2r$, $r\sqrt{3}$)

$(0, r, r\sqrt{3})$

$(0, -r, r\sqrt{3})$

$(r\sqrt{3}, 2r, r\sqrt{3})$

$(r\sqrt{3}, 0, r\sqrt{3})$

$(r\sqrt{3}, -2r, r\sqrt{3})$

$(-r\sqrt{3}, 2r, -r\sqrt{3})$

$(-r\sqrt{3}, 0, -r\sqrt{3})$

$(-r\sqrt{3}, -2r, -r\sqrt{3})$

$(0, r, -r\sqrt{3})$

$(0, -r, -r\sqrt{3})$

$(r\sqrt{3}, 2r, -r\sqrt{3})$

$(r\sqrt{3}, 0, -r\sqrt{3})$

$(r\sqrt{3}, -2r, -r\sqrt{3})$

All the co-ordinates above describe three rows of spheres layer.

Row of spheres layer: 17 .

Refractive index of Iodolyte TG50: 1.43 .

Refractive index of TiO_2 : 2.25 .

Material dispersion of TiO_2 : $\omega=3.1$, $\gamma=0.008$, $\delta\epsilon=0.1$.

Direction of wave propagation: positive x-direction .

Non-polarized source: summation of E_z , E_y , E_x continuous-src.

Angled source: resolve k-direction and amplitude $\exp(ikx)$.

Resolution: 30 .

Boundaries conditions: Bloch-periodic in z-directions and y-directions. Perfectly-matched layer (PML) is absorbing in x-directions.

PML Thickness: length of $5r$.

Padded air layer: distance of $15r$ between PML and materials.

Figure 1. 3D MayaVi visualization on TiO_2 inverse opal.

Figure 2. 2D slice of TiO_2 film and inverse opal bilayer.

Reference

1. Taflove, A.; Hagness, S. C. *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, Artech: Norwood, MA, **2000**.
2. Farjadpour, A.; Roundy, D.; Rodriguez, A.; Ibanescu, M.; Bermel, P.; Joannopoulos, J. D.; Johnson, S. G.; Burr, G. *Optics Letters* **2006**, 31 (20), 2972–2974.