Supporting information: Photonic approach in stacked slabs having periodic holes for enhancing photocatalytic activities

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S1. Design of antireflection for the stacked photonic crystal slabs

For the design of the antireflection region in the system of Fig. 2, we employ the impedance matching method presented in Ref. 1. First, we consider the transverse wave impedance $Z(z)$ along the z-axis, which is given by[2],

$$Z(z) = \begin{cases} -\dfrac{\iint_{(x,y)\in\Omega_{xy}} E_y(\boldsymbol{r})dxdy}{\iint_{(x,y)\in\Omega_{xy}} H_x(\boldsymbol{r})dxdy} & (\text{s}-\text{polarization}) \\ \\ \dfrac{\iint_{(x,y)\in\Omega_{xy}} E_x(\boldsymbol{r})dxdy}{\iint_{(x,y)\in\Omega_{xy}} H_y(\boldsymbol{r})dxdy} & (\text{p}-\text{polarization}) \end{cases}, \tag{S1}$$

where Ω_{xy} represents the area of the unit cell in the xy-plane. The antireflection condition satisfies

$$Z_h = \frac{Z_a^2}{Z_\text{S}}, \tag{S2}$$

$$\frac{(n_a - 1)D_a k_{z,a}}{2\pi} = \frac{2m-1}{4}, \tag{S3}$$

where Z_h and Z_a are the transverse impedances of the host photonic crystal region ($j = n_a$ to $N - n_a + 1$) and the antireflection photonic crystal regions ($j = 1$ to n_a and $j = N - n_a + 1$ to N), respectively, at the interfaces of each of the antireflection photonic crystal regions with the host photonic crystal region and the semi-infinite SiO_2 substrate. Z_S is the transverse impedance of the SiO_2 substrates, which has the forms of $Z_\text{S} = Z_0/\left(\sqrt{\varepsilon_\text{S}}\cos\theta\right)$ for s-polarization and $Z_\text{S} = Z_0\cos\theta/\sqrt{\varepsilon_\text{S}}$ for p-polarization, respetively, with Z_0 and θ being the free-space characteristic impedance and the incident angle from the z-axis. We have selected center-to-center distances $D_a = 1.29a$ and $D_h = 1.5a$ between neighboring photonic crystal slabs in the host and antireflection regions to satisfy Eq. (S2). In Eq. (S3), $k_{z,a}$ is the wavevector component along the z axis in the antireflection region and m is a positive integer. We have selected $n_a = 2$ to satisfy Eq. (S3), where the antireflection region has a quarter guided wavelength ($m = 1$). We note that the stacked photonic crystal in the antireflection region has been designed at $f_d' = 745$ THz in the analytical model of Fig. 2(d), which is 0.6 % lower than the design frequency $f_d = 749.5$ THz as shown in Fig. S1.

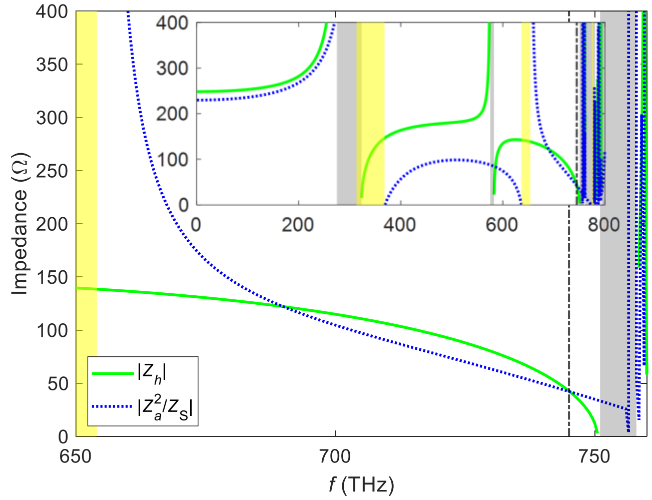

Fig.S1. Comparison of transverse impedance $|Z_h|$ for the host region (green solid line) and $|Z_a^2/Z_\mathrm{S}|$ coming from the antireflection condition (blue dotted line) in a frequency range from 650THz to 760THz, for $D_h = 1.5a$ and $D_a = 1.29a$. The vertical black dashed-dotted line represents frequency $f_d' = 745$ THz, which is 0.6% lower than design frequency $f_d = 749.5$THz. The shaded areas with gray and yellow denote bandgaps of the host region and the antireflection region, respectively. The inset shows the plots in a wide frequency range from 0 to 800THz.

S2. Fourier coefficient of the permittivity for the photonic crystal slab coated with photocatalyst layers

In the system of Fig. 2, where each photonic crystal slab has photocatalyst layers at both sides, the Fourier coefficient of the permittivity is given by

$$\mathcal{E}(\boldsymbol{g}-\boldsymbol{g}') = \begin{cases} \varepsilon_\mathrm{w} + (\varepsilon_\mathrm{w}-\varepsilon_\mathrm{c})\left(\dfrac{\pi R^2}{a^2}-1\right)\dfrac{t_K+2t_c}{D} + (\varepsilon_\mathrm{c}-\varepsilon_\mathrm{K})\left(\dfrac{\pi R^2}{a^2}-1\right)\dfrac{t_K}{D} & (\Delta\boldsymbol{g}_{xy}=\boldsymbol{0},\ \Delta g_z=0) \\ 2(\varepsilon_\mathrm{w}-\varepsilon_\mathrm{c})\dfrac{\pi R^2}{a^2}\left(\dfrac{t_K+2t_c}{D}\right)\dfrac{J_1(|\Delta\boldsymbol{g}_{xy}|R)}{|\Delta\boldsymbol{g}_{xy}|R} + 2(\varepsilon_\mathrm{c}-\varepsilon_\mathrm{K})\dfrac{\pi R^2}{a^2}\dfrac{t_K}{D}\dfrac{J_1(|\Delta\boldsymbol{g}_{xy}|R)}{|\Delta\boldsymbol{g}_{xy}|R} & (\Delta\boldsymbol{g}_{xy}\neq\boldsymbol{0},\ \Delta g_z=0) \\ (\varepsilon_\mathrm{w}-\varepsilon_\mathrm{c})\left(\dfrac{\pi R^2}{a^2}-1\right)\left(\dfrac{t_K+2t_c}{D}\right)\dfrac{\sin(\Delta g_z(t_K+2t_c)/2)}{\Delta g_z(t_K+2t_c)/2} + (\varepsilon_\mathrm{c}-\varepsilon_\mathrm{K})\left(\dfrac{\pi R^2}{a^2}-1\right)\dfrac{t_K}{D}\dfrac{\sin(\Delta g_z t_K/2)}{\Delta g_z t_K/2} & (\Delta\boldsymbol{g}_{xy}=\boldsymbol{0},\ \Delta g_z\neq 0) \\ 2(\varepsilon_\mathrm{w}-\varepsilon_\mathrm{c})\dfrac{\pi R^2}{a^2}\left(\dfrac{t_K+2t_c}{D}\right)\dfrac{J_1(|\Delta\boldsymbol{g}_{xy}|R)}{|\Delta\boldsymbol{g}_{xy}|R}\dfrac{\sin(\Delta g_z(t_K+2t_c)/2)}{\Delta g_z(t_K+2t_c)/2} + 2(\varepsilon_\mathrm{c}-\varepsilon_\mathrm{K})\dfrac{\pi R^2}{a^2}\dfrac{t_K}{D}\dfrac{J_1(|\Delta\boldsymbol{g}_{xy}|R)}{|\Delta\boldsymbol{g}_{xy}|R}\dfrac{\sin(\Delta g_z t_K/2)}{\Delta g_z t_K/2} & (\Delta\boldsymbol{g}_{xy}\neq\boldsymbol{0},\ \Delta g_z\neq 0) \end{cases}, \quad \text{(S4)}$$

where $D = D_h$ for the host region and $D = D_a$ for the antireflection region, respectively, $\Delta\boldsymbol{g}_{xy} = (g_x - g_x',\ g_y - g_y'),\Delta g_z = g_z - g_z'$, and J_1 represents the Bessel function of the first kind.

S3. Derivation of Eqs. (5) and (6)

We start with Maxwell's equations

$$\begin{cases} \nabla \times \boldsymbol{E}(\boldsymbol{r}) = i\omega\mu_0 \boldsymbol{H}(\boldsymbol{r}) \\ \nabla \times \boldsymbol{H}(\boldsymbol{r}) = -i\omega\varepsilon_0\varepsilon(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r}) \end{cases}. \tag{S5}$$

Substituting Eqs. (2)-(4) into (S5), we have

$$\begin{cases} \boldsymbol{h}_g = \dfrac{c_0}{\omega}(\boldsymbol{k}+\boldsymbol{g}) \times \boldsymbol{e}_G \\ \boldsymbol{e}_g = -\dfrac{c_0}{\omega}\displaystyle\sum_{\boldsymbol{g}'} \mathcal{E}^{-1}(\boldsymbol{g}-\boldsymbol{g}')(\boldsymbol{k}+\boldsymbol{g}') \times \boldsymbol{h}_{g'} \end{cases}, \tag{S6}$$

where c_0 represents the speed of light in vacuum. In the case of the normal incidence $(k_x, k_y) = (0,0)$, each component of Eq. (S6) is described as

$$\begin{cases} g_y e_{z,g} - (k_z + g_z)e_{y,g} = \dfrac{\omega}{c_0} h_{x,g} \\ (k_z + g_z)e_{x,g} - g_x e_{z,g} = \dfrac{\omega}{c_0} h_{y,g} \\ g_x e_{y,g} - g_y e_{x,g} = \dfrac{\omega}{c_0} h_{z,g} \\ \displaystyle\sum_{\boldsymbol{g}'} \mathcal{E}^{-1}(\boldsymbol{g}-\boldsymbol{g}')\{g'_y h_{z,g'} - (k_z + g'_z)h_{y,g'}\} = -\dfrac{\omega}{c_0} e_{x,g} \\ \displaystyle\sum_{\boldsymbol{g}'} \mathcal{E}^{-1}(\boldsymbol{g}-\boldsymbol{g}')\{(k_z + g'_z)h_{x,g'} - g'_x h_{z,g'}\} = -\dfrac{\omega}{c_0} e_{y,g} \\ \displaystyle\sum_{\boldsymbol{g}'} \mathcal{E}^{-1}(\boldsymbol{g}-\boldsymbol{g}')\{g'_x h_{y,g'} - g'_y h_{x,g'}\} = -\dfrac{\omega}{c_0} e_{z,g} \end{cases}. \tag{S7}$$

Equation (S7) is rewritten in the matrix form as

$$\begin{cases} -\boldsymbol{G}_z\boldsymbol{e}_x + \dfrac{c_0}{\omega}\boldsymbol{G}_x\boldsymbol{\mathcal{E}}^{-1}\boldsymbol{G}_y\,\boldsymbol{h}_x - \dfrac{c_0}{\omega}\left\{\boldsymbol{G}_x\boldsymbol{\mathcal{E}}^{-1}\boldsymbol{G}_x - \left(\dfrac{\omega}{c_0}\right)^2\right\}\boldsymbol{h}_y = k_z\boldsymbol{e}_x \\ -\boldsymbol{G}_z\boldsymbol{e}_y + \dfrac{c_0}{\omega}\left\{\boldsymbol{G}_y\boldsymbol{\mathcal{E}}^{-1}\boldsymbol{G}_y - \left(\dfrac{\omega}{c_0}\right)^2\right\}\boldsymbol{h}_x - \dfrac{c_0}{\omega}\boldsymbol{G}_y\boldsymbol{\mathcal{E}}^{-1}\boldsymbol{G}_x\,\boldsymbol{h}_y = k_z\boldsymbol{e}_y \\ -\dfrac{c_0}{\omega}\boldsymbol{G}_x\,\boldsymbol{G}_y\boldsymbol{e}_x - \dfrac{c_0}{\omega}\left\{\left(\dfrac{\omega}{c_0}\right)^2\boldsymbol{\mathcal{E}} - \boldsymbol{G}_x\,\boldsymbol{G}_x\right\}\boldsymbol{e}_y - \boldsymbol{G}_z\,\boldsymbol{h}_x = k_z\boldsymbol{h}_x \\ \dfrac{c_0}{\omega}\left\{\left(\dfrac{\omega}{c_0}\right)^2\boldsymbol{\mathcal{E}} - \boldsymbol{G}_y\,\boldsymbol{G}_y\right\}\boldsymbol{e}_x + \dfrac{c_0}{\omega}\boldsymbol{G}_y\,\boldsymbol{G}_x\boldsymbol{e}_y - \boldsymbol{G}_z\,\boldsymbol{h}_y = k_z\boldsymbol{h}_y \\ \dfrac{c_0}{\omega}\boldsymbol{\mathcal{E}}^{-1}\boldsymbol{G}_y\,\boldsymbol{h}_x - \dfrac{c_0}{\omega}\boldsymbol{\mathcal{E}}^{-1}\boldsymbol{G}_x\,\boldsymbol{h}_y = \boldsymbol{e}_z \\ -\dfrac{c_0}{\omega}\boldsymbol{G}_y\boldsymbol{e}_x + \dfrac{c_0}{\omega}\boldsymbol{G}_x\boldsymbol{e}_y = \boldsymbol{h}_z \end{cases}. \tag{S8}$$

Eq. (5) is given from the 1st line to the 4th line of Eq. (S8), and Eq. (6) is given from the 5th line and the 6th line of Eq. (S8).

S4. Calculation method for transmission, reflection, and absorption of the analytical model

Fresnel reflection and transmission coefficients at the interface of the lth medium and the $l+1$th medium in the analytical model of Fig. 2(d) are given by

$$r_{l,l+1} = \begin{cases} \dfrac{Z_{l+1} - Z_l}{Z_{l+1} + Z_l} & (\mathrm{s-polarization}) \\ \dfrac{Z_l - Z_{l+1}}{Z_l + Z_{l+1}} & (\mathrm{p-polarization}) \end{cases}, \tag{S9}$$

$$t_{l,l+1} = \begin{cases} \dfrac{2Z_{l+1}}{Z_{l+1} + Z_l} & (\mathrm{s-polarization}) \\ \dfrac{2Z_l}{Z_l + Z_{l+1}} & (\mathrm{p-polarization}) \end{cases}. \tag{S10}$$

Electric fields E_1^+ and E_1^- in the 1st medium and electric fields E_5^+ and E_5^- in the 5th medium, where the superscripts + and – denote the forward and backward directions along the z axis, are related by the transfer matrix method[3]

$$\begin{bmatrix} E_5^+ \\ E_5^- \end{bmatrix} = \boldsymbol{M}_{54}\boldsymbol{\Phi}_4\boldsymbol{M}_{43}\boldsymbol{\Phi}_3\boldsymbol{M}_{32}\boldsymbol{\Phi}_2\boldsymbol{M}_{21}\begin{bmatrix} E_1^+ \\ E_1^- \end{bmatrix}, \tag{S11}$$

where

$$\boldsymbol{M}_{l+1,l} = \begin{bmatrix} t_{l,l+1} - \dfrac{r_{l,l+1}r_{l+1,l}}{t_{l+1,l}} & \dfrac{r_{l+1,l}}{t_{l+1,l}} \\ -\dfrac{r_{l,l+1}}{t_{l+1,l}} & \dfrac{1}{t_{l+1,l}} \end{bmatrix}, \tag{S12}$$

$$\boldsymbol{\Phi}_l = \begin{bmatrix} \exp(ik_{z,l}h_l) & 0 \\ 0 & \exp(-ik_{z,l}h_l) \end{bmatrix}. \tag{S13}$$

The propagation length is $h_l = (N - 2n_a + 1)D_h$ for the host region $(l = 3)$ and $h_l = (n_a - 1)D_a$ for the antireflection region $(l = 2,4)$. We note that $k_{z,l}$ is complex for the host region $(l = 3)$ and the antireflection region $(l = 2,4)$. Reflection R, transmission T, and absorption A of the analytic model are expressed as

$$R = |E_1^-/E_1^+|^2, \tag{S14}$$

$$T = |E_5^+/E_1^+|^2, \tag{S15}$$

$$A = 1 - R - T. \tag{S16}$$

S5. Absorption spectra for various N obtained from the analytic model

We obtain the absorption spectra for various N of the photonic crystal slabs in the host region, from the analytical model of Fig.2(d), as shown in Fig. S2. The analytical result of Fig.S2 agrees well with the numerical result of Fig. 5(b).

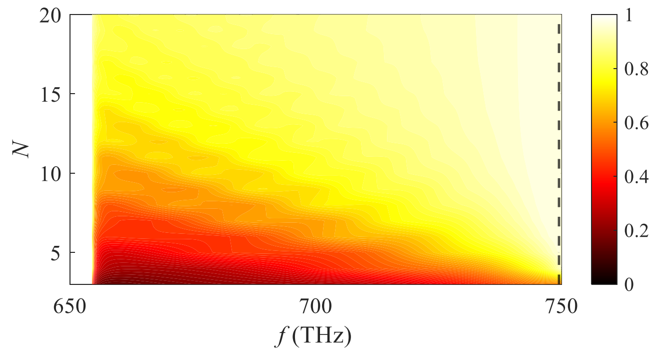

Fig. S2 Absorption spectra for various N of the photonic crystal slabs obtained from the analytic model of Fig.2(d). The white region around 650THz represents the band gap of the photonic crystal slabs.

References

1. H. Iizuka, N. Engheta and S. Sugiura, *Opt Lett*, 2016, **41**, 3829-3832.
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3. B. E. Saleh and M. C. Teich, *Fundamentals of photonics*, john Wiley & sons, Second Edition edn., 2007.