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Supporting Information

Small Band Gap Conjugated Polyelectrolytes for Photothermal Killing of Bacteria

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Calculation of Photothermal Conversion Efficiency

Following Roper's report,^{1,2} the total balance of the system can be expressed:

$$\sum_{i} m_i C_{p,i} \frac{dT}{dt} = Q_{CPE} + Q_{Dis} - Q_{surr}$$
⁽¹⁾

where m_i and $C_{p,i}$ are the mass and heat capacity of water. T is the solution temperature, Q_{CPE} is the energy inputted by CPE. Q_{Dis} is the energy input by the sample cells, Q_{surr} is heat conduction away to the air.

The laser induced energy, Q_{CPE} represent the heat dissipated by electron-phonon relaxation.

$$Q_{CPE} = I(1 - 10^{A_{808}})\eta$$
⁽²⁾

Where I is laser power, η is photothermal conversion efficiency. A808 is the absorbance of CPE at 808 nm. In addition, the heat dissipated from the sample cell, Q_{Dis} is measured to be 14.5 mW using pure water as control.

The energy transfer to air is:

$$Q_{surr} = hS(T - T_{surr}) \tag{3}$$

Where h is heat transfer coefficient, S is the surface area. T_{surr} is the ambient temperature.

As the heat input Q_{CPE} and Q_{Dis} is based on laser input, the Q_{surr} increase with temperature increase. Under laser irradiation, the temperature of the system increases to equilibrium, where the temperature is defined as T_{max} . When temperature reach T_{max} , the input is equal to heat output.

$$Q_{CPE} + Q_{Dis} = hS(T_{max} - T_{surr})$$
⁽⁴⁾

To get hS, a dimensionless drive force temperature is defined as

$$\theta = \frac{T - T_{surr}}{T_{max} - T_{surr}}$$
(5)

and a sample system time constant is defined as

$$\tau_s = \frac{\sum m_i C_{p,i}}{hS} \tag{6}$$

Combine Eq (1) and (6)

$$\frac{d\theta}{dt} = \frac{1}{\tau_s} \left(\frac{Q_{CPE} + Q_{Dis}}{hS(T_{max} - T_{surr}} - \theta) \right)$$
(7)

At the cooling stage as shown in Figure 1A, laser input is shut off, and $Q_{CPE} + Q_{Dis} = 0$, and hence Eq (7) becomes

$$t = -\tau_s(\ln\theta) \tag{8}$$

From Figure S2 plot, τ_s is calculated to be 201 s, and 182 s for **P1** and **P2**, respectively, which is used to calculate hS. As laser output area is 0.5 cm², the photothermal conversion efficiency is calculated to be 33.2% and 32.0% for **P1**, and **P2**, respectively.



Figure S1. ROS generation of **P1** and **P2** under irradiation using ABDA as the indicator. A) Absorbance change of ABDA at 400 nm in the present of **P1** or **P2** under irradiation. Absorbance spectra of B)ABDA solution, C) ABDA and **P1** solution, D) ABDA and **P2** solution, under irradiaiton.



Figure S2. A) Temperature changes of CPE aqueous solution (50 μ g/mL), in which the laser lasts for 10 min, and then the laser is switched off. B) Plot of linear time data

from the cooling stage versus negative natural logarithm of drive force temperature. The slop represents the sample system time constant τ_s .



Figure S3. A) Absorption spectra of Van A before and after treatment with **P1** or **P2** (100 μ g/mL). B) Zeta potential changes of Van A after treatment with **P1** or **P2** at different concentrations.



Figure S4. A) Absorption spectra of Van B before and after treatment with **P1** or **P2** (100 μ g/mL). B) Zeta potential changes of Van B after treatment with **P1** or **P2** at different concentrations.



Figure S5. A) Absorption spectra of *B. Subtilis* after treatment with A) **P1** or B) **P2** at different concentrations. C) Plot of absorbance at 750 nm versus **P1** or **P2** at different concentrations. D) Zeta potential changes of *B. Subtilis* after treatment with **P1** or **P2** at different concentrations.



Figure S6. A) Absorption spectra and B) zeta potential changes of HeLa cells before and after treatment with P1 or P2 (100 μ g/mL).



Figure S7. Plate photographs for *E coli* LB agar plate supplemented with **P1** under dark (A, B, C) and upon 808 nm laser irradiation (0.75 W/cm² for 6 min) (C, D, E). The concentrations of **P1** used for incubation are 10 (A, D), 20 (B, E) and 100 (C, F) μ g/mL.



Figure S8. Plate photographs for *B. subtilis* LB agar plate supplemented with **P1** under dark (A, B, C) and upon 808 nm laser irradiation (0.75 W/cm² for 6 min) (C, D, E). The concentrations of **P1** used for incubation are 10 (A, D), 20 (B, E) and 100 (C, F) μ g/mL.



Figure S9. A) CFU survival percentages and B) photographs of Van A LB agar plate supplemented with **P1** in dark and upon 808 nm laser irradiation (0.75 W/cm² for 6 min).



Figure S10. A) CFU survival percentages and B) photographs of Van B LB agar plate supplemented with **P1** in dark and upon 808 nm laser irradiation (0.75 W/cm² for 6 min).



Figure S11. Plate photographs for *E coli* LB agar plate supplemented with **P2** under dark (A, B, C) and upon 808 nm laser irradiation (0.75 W/cm² for 6 min) (C, D, E). The concentrations of **P2** used for incubation are 10 (A, D), 20 (B, E) and 100 (C, F) μ g/mL.



Figure S12. Plate photographs for *B. Subtilis* LB agar plate supplemented with **P2** under dark (A, B, C) and upon 808 nm laser irradiation (0.75 W/cm² for 6 min) (C, D, E). The concentrations of **P2** used for incubation are 10 (A, D), 20 (B, E) and 100 (C, F) μ g/mL, respectively.

References

(1) Roper, D. K.; Ahn, W.; Hoepfner, M. *The Journal of Physical Chemistry C* **2007**, *111*, 3636.

(2) Tian, Q.; Jiang, F.; Zou, R.; Liu, Q.; Chen, Z.; Zhu, M.; Yang, S.; Wang, J.; Wang, J.; Hu, J. *ACS Nano* **2011**, *5*, 9761.