Carbon-based nanomaterials with greater specific surface area are more expensive but more effective at antimicrobials

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Supplementary data

Table S1. C, O, N and Zn content in NPC-T obtained by XPS analysis.

	C atom ratio (at%)	O atom ratio (at%)	N atom ratio (at%)	Zn atom ratio (at%)
NPC-600	69.25	12.35	17.13	1.27
NPC-700	69.86	9.23	19.5	1.42
NPC-800	69.7	8.46	20.17	1.66
NPC-900	75.07	8.47	15.04	1.42
NPC-1000	83.37	10.72	5.64	0.26

Table S2. Zn content in NPC-T obtained by EDS analysis.

Sample	Weight ratio (wt%)	Atomic ratio (at%)
NPC-600	2.94	0.66
NPC-700	0.74	0.15
NPC-800	2.96	0.62
NPC-900	2.4	0.51
NPC-1000	1.04	0.22

Table S3. Zn content in NPC-T obtained by ICP-OES analysis.

Sample	Mean (mg/L)
NPC-600	121.4
NPC-700	157.1
NPC-800	197.5
NPC-900	146.8
NPC-1000	102.3

Table S4. Specific surface area, cumulative pore volume and pore size of NPC-T.

sample	BET specific surface area (m^2/g)	Pore volume (cm^3/g)	Pore size (nm)
NPC-600	64.7936	0.372662	34.5756
NPC-700	691.3567	0.546245	16.0580
NPC-800	771.1273	0.722642	21.7783
NPC-900	811.4681	0.771971	27.7232
NPC-1000	994.5579	0.829571	27.4536

Table S5. The absorbance at 652nm of different samples after catalase like reaction at different temperatures

sample	25℃ (OD Value a.u.)	37℃ (OD Value a.u.)	45℃ (OD Value a.u.)	50℃ (OD Value a.u.)	55℃ (OD Value a.u.)
NPC-600	0.2963	0.2976	0.4151	0.4702	0.5442
NPC-700	0.4987	0.5176	0.7879	0.7884	0.9966
NPC-800	0.6076	0.6998	0.9267	1.0621	1.136
NPC-900	1.0473	1.213	1.4885	1.6038	1.6062
NPC-1000	1.4215	1.5032	1.6043	1.7022	1.7807

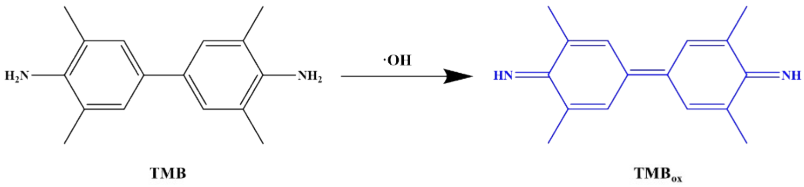

Figure S1. Chemical formula for the reaction of TMB with ·OH to form the blue TMB oxide.

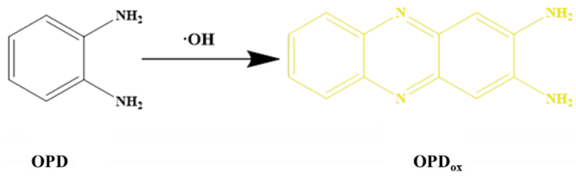

Figure S2. Chemical formula for the reaction of OPD with ·OH to form the yellow OPD oxide.

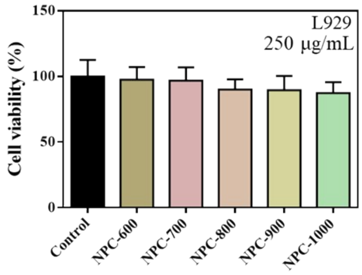

Figure S3. Cell viability of L929 treated with 250 μg/mL NPC-T.

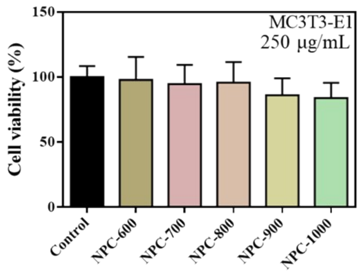

Figure S4. Cell viability of MC3T3-E1 treated with 250 μg/mL NPC-T.

Calculation of the photothermal conversion efficiency[1]:

$$\sum_i m_i C_i \frac{dT}{dt} = Q_P + Q_W + Q_L \quad (1)$$

Equation (1) is the energy balance equation of the system. Where m_i and C_i are the mass and specific heat capacity of NPC-T dispersion, T is the temperature of NPC-T dispersion, t is the laser irradiation time, Q_P is the heat generated by the photothermal conversion of NPC-T under laser irradiation, Q_W is the heat generated by the photothermal conversion of water under laser irradiation, and Q_L is the heat flowing from the system to the surrounding environment.

$$Q_P = I\left(1 - 10^{-A_{808}}\right)\eta \quad (2)$$

In Equation (2), I is the laser power input to the system, A_{808} is the absorbance of the NPC-T at 808 nm, and η is the photothermal conversion efficiency of the NPC-T.

$$Q_L = hS\Delta T \quad (3)$$

In Equation (3), h is the heat transfer coefficient, S is the area of the laser spot, $\Delta T = T - T_{surr}$, T is the real-time temperature of the system, and T_{surr} is the ambient temperature.

When the system temperature reaches equilibrium, the heat generated by the photothermal conversion is equal to the heat dissipated, at this time:

$$Q_P + Q_W = Q_L = hS\Delta T_{max} \quad (4)$$

In Equation (4), ΔT_{max} is the value of temperature change when the system is in equilibrium, and according from Equation (2-4), the formula for the photothermal conversion efficiency can be obtained:

$$\eta = \frac{hS\Delta T_{max} - Q_W}{I(1 - 10^{-A_{808}})} \quad (5)$$

In Equation (5), the parameter hS is unknown, so θ can be introduced to find hS, and θ is defined as:

$$\theta = \frac{\Delta T}{\Delta T_{max}} \quad (6)$$

Equation (3) and Equation (6) are brought into Equation (1) to derive Equation (7):

$$\frac{d\theta}{dt}=\frac{hS}{\sum_i m_iC_i}\left(\frac{Q_P+Q_W}{hS\Delta T_{max}}-\theta\right) \quad (7)$$

When the laser is turned off, the system cools down naturally, and at this stage Q_P+Q_W=0. Equation (7) can be derived as:

$$t=-\frac{\sum_i m_iC_i}{hS}ln\theta=-\tau_s ln\theta \quad (8)$$

where τ_s is the time dosage of the system and denotes the slope of the line between time t and -lnθ. Considering that the mass of NPC-T in the NPC suspension is 1 mg, which is much smaller than the mass of water (1 g), and secondly, m_PC_P can be neglected because of the specific heat capacity of water is larger than that of NPC-T. Due to the linear relationship between the system's natural cooling phase, t, and $-ln\theta$, it is possible to find hS.

$$hS=\frac{m_WC_W}{\tau_s} \quad (9)$$

Q_W in Equation (5) can be found by the warming process of laser irradiation of deionized water with the following equation:

$$Q_W=\frac{m_WC_W\Delta T_{max,H_2O}}{\tau_s} \quad (10)$$

In Equation (10), m_W is the mass of deionized water, C_W is the specific heat capacity of deionized water, $\Delta T_{max,H_2O}$ is the temperature change of laser irradiation of deionized water to reach the equilibrium of the system, and τ_s is the time usage of the system.

Therefore, the photothermal conversion efficiency of NPC-T dispersion can be calculated according to Equation (5) and Equations (8-10).

$$\eta=\frac{hS(\Delta T_{max}-\Delta T_{max,H_2O})}{I(1-10^{-A_{808}})} \quad (11)$$

In the above equation, hS = 0.01376 W °C^{-1}, τ_s = 305.175 s, m = 1 g, C = 4.2 J g^{-1}, I = 1 W cm^{-2}, and A_{808} = 0.2765.

Reference

[1] Liu Y, Ai K, Liu J, et al. Dopamine-melanin colloidal nanospheres: An efficient near-infrared photothermal therapeutic agent for in vivo cancer therapy[J]. Advanced Materials, 2013, 25(9): 1353-1359.