Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Support information

HKUST-1 Loaded Few-layer $Ti_3C_2T_x$ for Synergistic Chemo-Photothermal Effects to Enhance Antibacterial Activity

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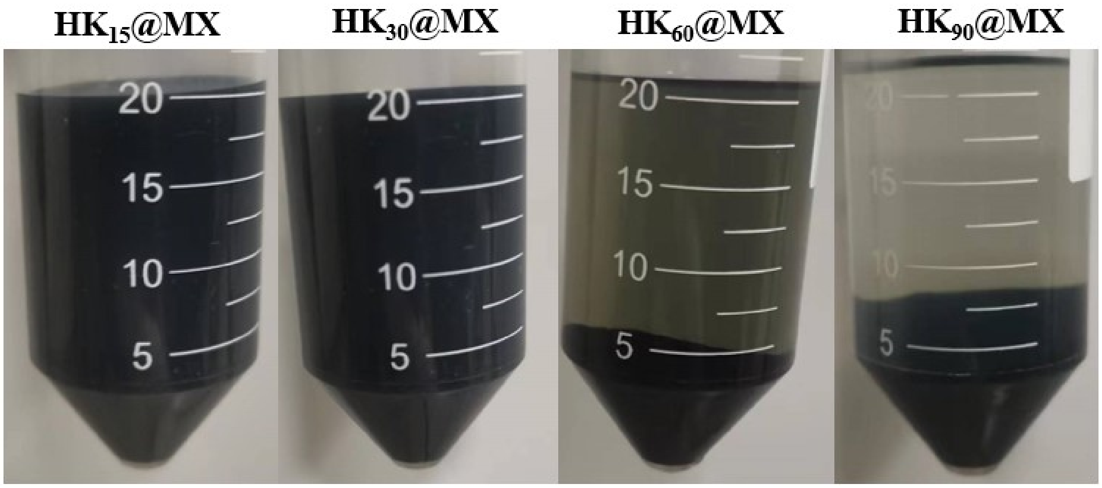

Figure S1 After the synthesis reaction, HK_{15}@MX, HK_{30}@MX, HK_{60}@MX and HK_{90}@MX were centrifuged in 2000 rmp/min for 5 minutes. The supernatant is getting cleaner while increase the loading of HKUST-1 on the surface of $Ti_3C_2T_x$. The high content of HKUST-1 on the surface of $Ti_3C_2T_x$ leads to the mass increase and deposition to the bottom.

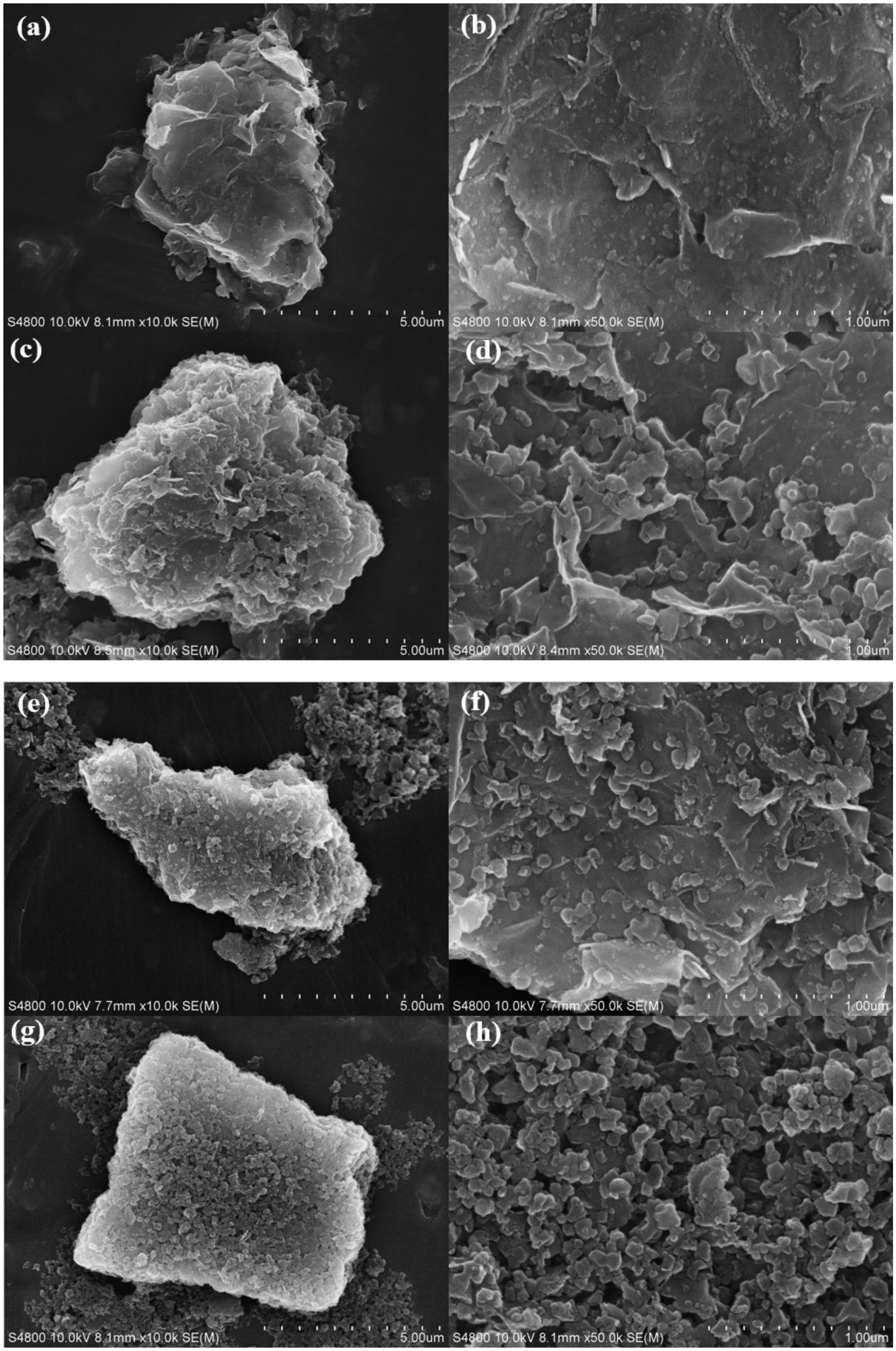

Figure S2. SEM images of (a-b) $HK_{15}@Ti_3C_2T_x$, (c-d) $HK_{30}@Ti_3C_2T_x$, (e-f) $HK_{60}@Ti_3C_2T_x$, (g-h) $HK_{90}@Ti_3C_2T_x$.

Table S1 Comparison of specific surface area and pore volume of $Ti_3C_2T_x$ and HK@MX samples

Materials	BET Surface Area ($m^2 \cdot g^{-1}$)	Pore volume ($cm^3 \cdot g^{-1}$)
$Ti_3C_2T_x$	11.748	2.68
HK_{15}@MX	57.226	13.157
HK_{30}@MX	109.45	25.149
HK_{60}@MX	131.03	30.105
HK_{90}@MX	186.76	42.908

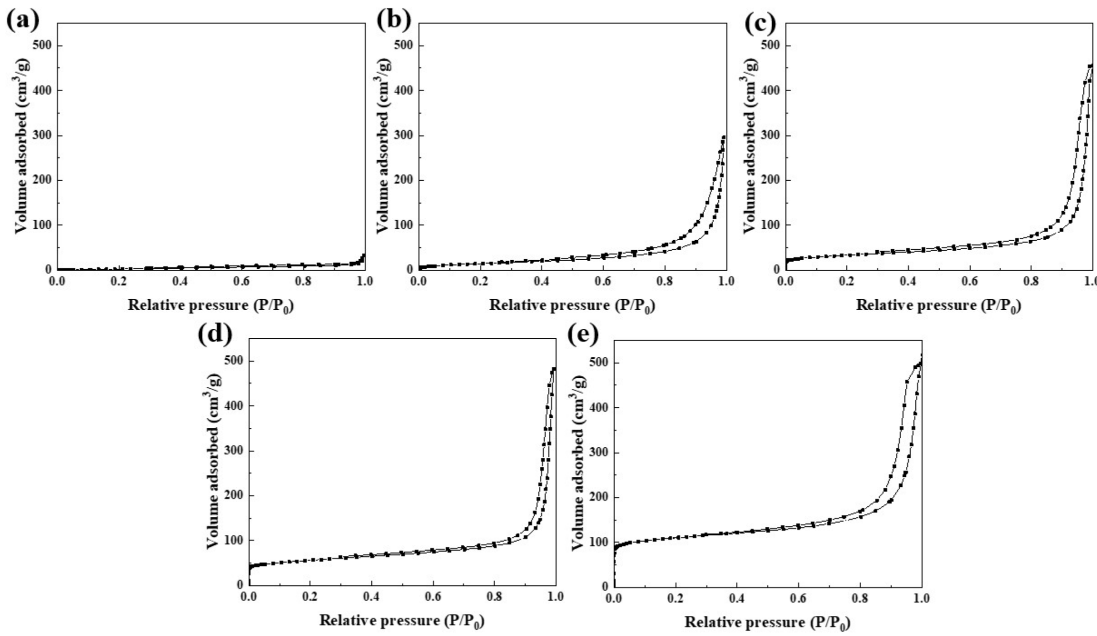

Figure S3 Nitrogen absorption–desorption isotherms of (a) $Ti_3C_2T_x$, (b) HK_{15}@$Ti_3C_2T_x$, (c) HK_{30}@$Ti_3C_2T_x$, (d) HK_{60}@$Ti_3C_2T_x$.and (e) HK_{90}@$Ti_3C_2T_x$.

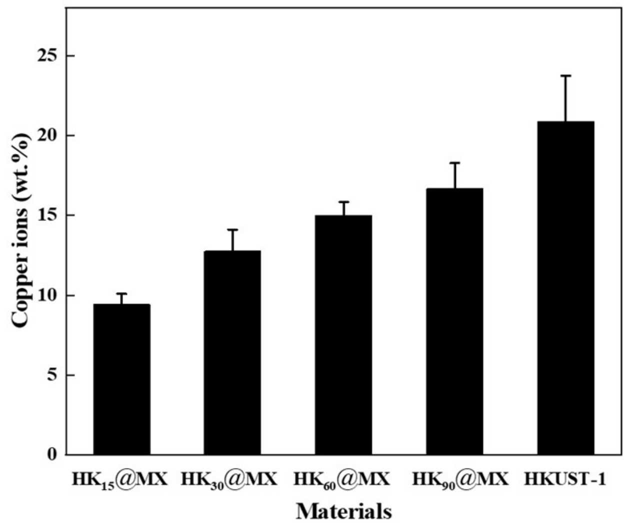

Figure. S4. ICP-MS analysis of Cu content in HKUST-1, HK_{15}@MX, HK_{30}@MX, HK_{60}@MX and HK_{90}@MX. (Calculation formula for measuring Cu element content= instrument reading × dilution factor × constant volume / sample quality. 10000 mg/kg = 1%.)

Photothermal performance of HK@MX

To evaluate the photothermal properties, a near-infrared laser (808 nm, 2 W cm^{-2}) was used to irradiate deionized water and HK@MX nanoparticles at different concentrations for 10 minutes. Dispersion temperature was monitored by a type K thermocouple (OMEGA HH309A, OMEGA Engineering Inc., Norwalk, CT, USA). To calculate the photothermal conversion efficiency of HK@MX nanoparticles, 2 mL HK@MX nanoparticle aqueous dispersion (200μg mL^{-1}) was irradiated continuously under the same conditions until the steady-state temperature was reached. Turn off the laser and record the temperature drop process. The photothermal conversion efficiency (η) is calculated by equation (1) described by literature[1]:

$$\eta = \frac{hS(T_{max} - T_{surr}) - Q_s}{I\left(1 - 10^{-A_{808}}\right)} \qquad (1)$$

Where, h is the heat transfer coefficient, S is the surface area of the container, T_{max} is the maximum system temperature, T_{surr} is the ambient temperature, Qs is the heat related to the optical absorbance of the solvent, I is the laser power (2 W cm^{-2}), and A808 is the absorbance at HK_{60}@MX at 808 nm. The value of hS is derived from equation (2)

$$\tau_S = \frac{m_D C_D}{hS} \qquad (2)$$

Including τ_S for sample system time constant, m_D and C_D respectively deionized water (1 g), and the quality of the heat capacity (4.2 J (g ℃)$^{-1}$). The Q_s value measured independently using pure water was 13.4 mW.

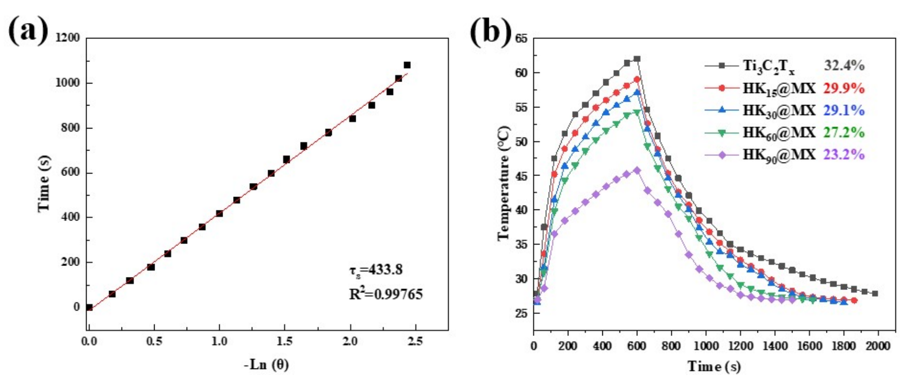

Figure. S5. (a) The fitting linear curve of time data vs -lnθ from the cooling period of HK_{60}@MX. (b) The heating/cooling curves of different nanoparticles with different HKUST-1 doping concentration under laser on/off.

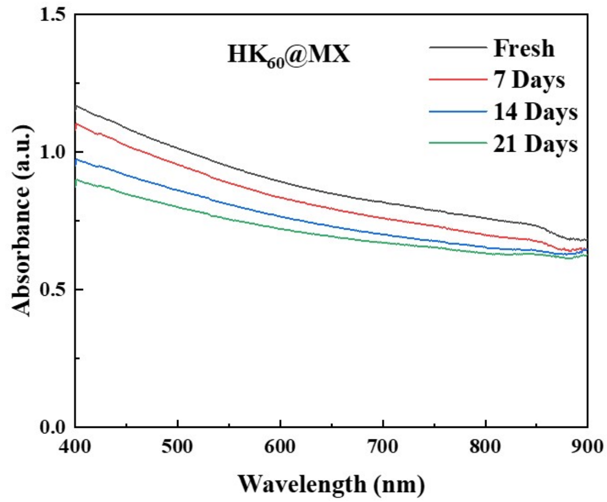

Figure. S6. Absorbance change of HK_{60}@MX dispersions in DI water for 21 days.

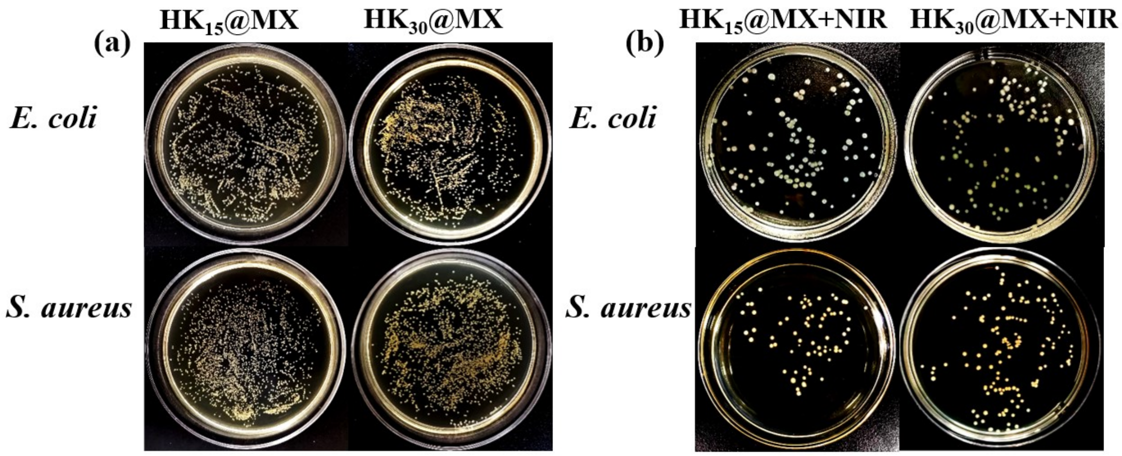

Figure S7 In vitro antibacterial activities of HK_{15}@MX and HK_{30}@MX against *S. aureus* and *E. coli.* (a) kept in the dark for 10 min (200 μg/ml) (b)exposed to 808 nm light (2 W/cm^2) for 10 min

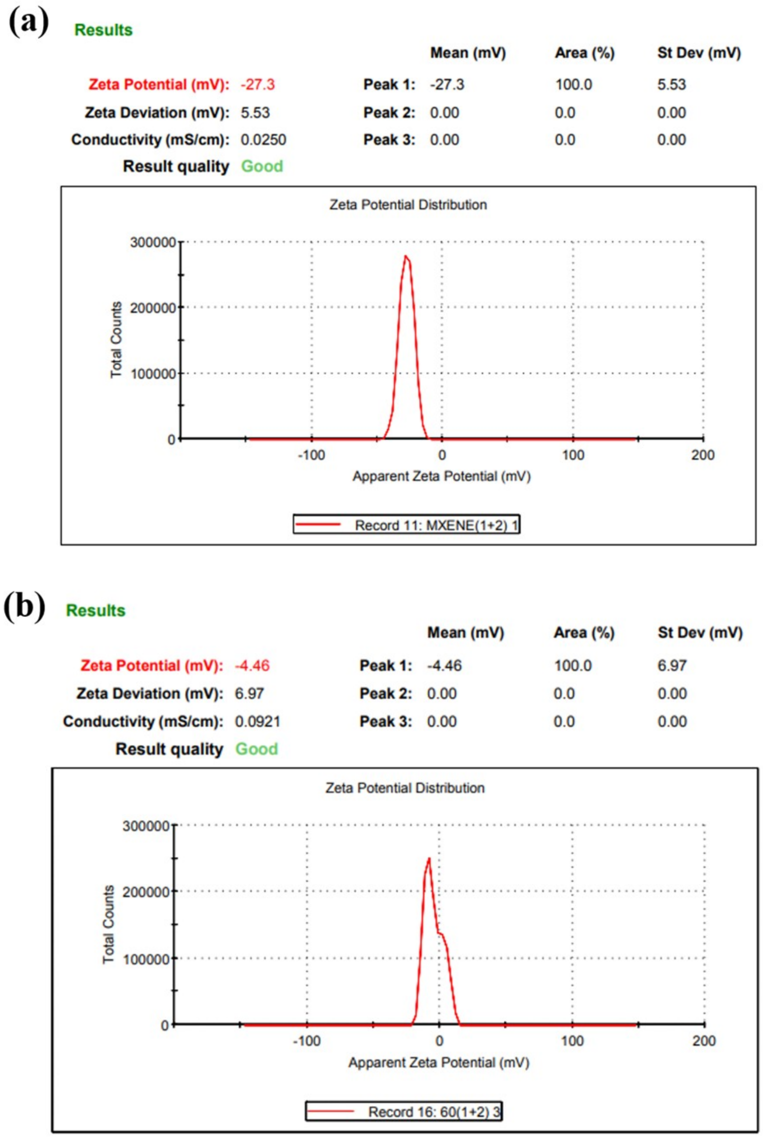

Figure S8 Distribution of zeta potential of (a)$Ti_3C_2T_x$ and (b)HK_{60}@MX at pH 7.5

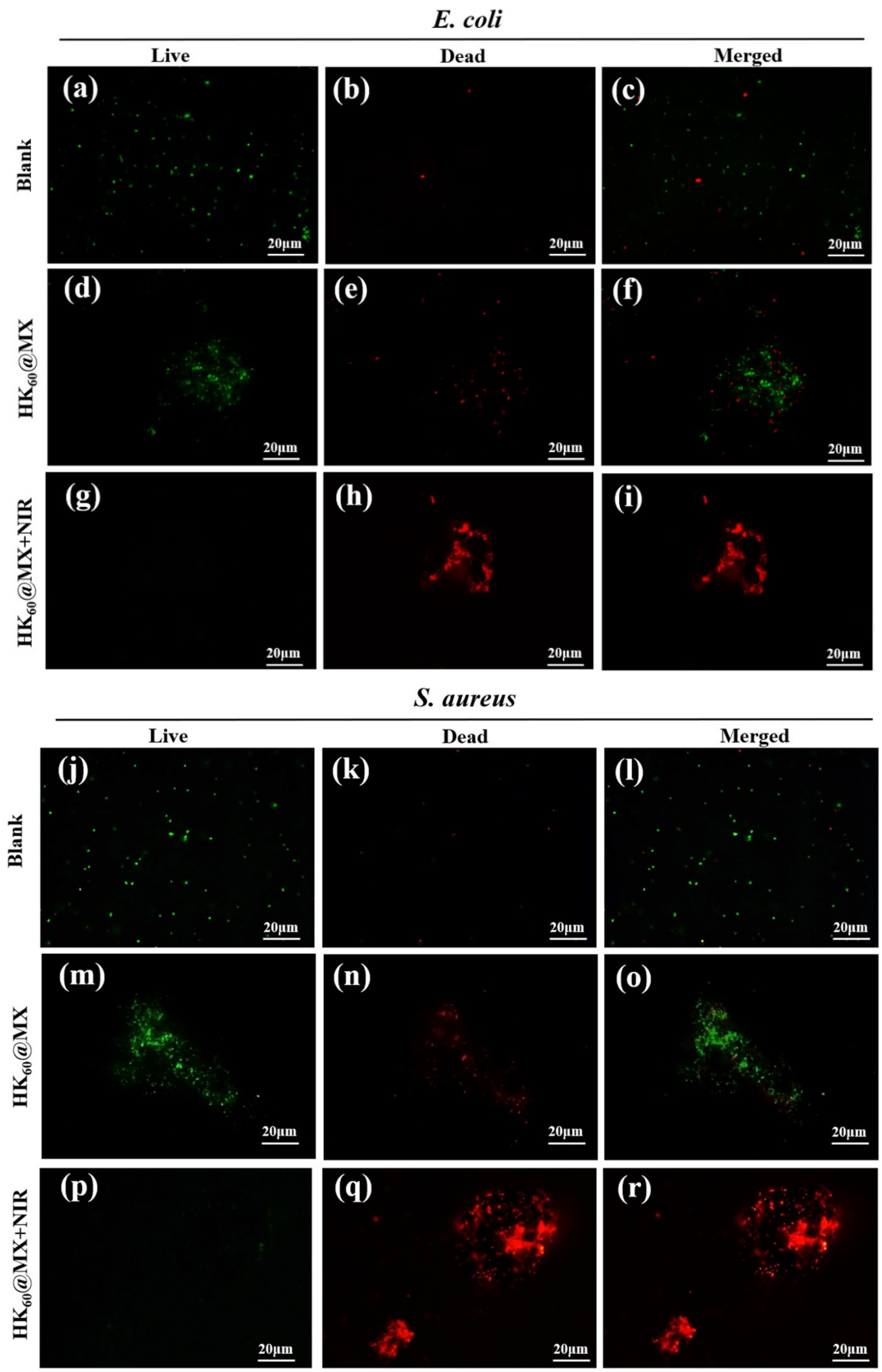

Figure S9. Confocal laser scanning microscopy (CLSM) images of E. coli (a-i) and S. aureus (j-r) treated with Meilungreen and PI staining. (a–c, j-l) control; (d–f, m-o) 200 μg/mL HK_{60}@MX; (g–i, p-r) 200μg/mL HK_{60}@MX+NIR.

Notes and references

1. Z. Chu, T. Tian, Z. Tao, J. Yang, B. Chen, H. Chen, W. Wang, P. Yin, X. Xia, H. Wang and H. Qian, *Bioactive Materials*, 2022, **17**, 71-80.