Supplementary information

Near infrared photothermal-responsive poly(vinyl alcohol)/black phosphorus composite hydrogels with excellent on-demand drug release capacity

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1. Calculation of the photothermal conversion efficiency

The photothermal conversion efficiency (η) of composite hydrogel was measured by a method reported by Roper and Wang, where η can be calculated using the following equations^{1, 2}:

$$\eta = \frac{hS(T_{max} - T_{surr}) - Q_{dis}}{I(1 - 10^{-A_{808}})}$$
(1)

In this equation, *h* is heat transfer coefficient, *S* is the surface area of the container. T_{max} is the equilibrium temperature, T_{surr} is ambient temperature of the surroundings, and $(T_{max} - T_{surr})$ was 28.6 °C according to Figure 7(c). Q_{dis} expresses heat dissipated from light absorbed by the quartz sample cell itself, and it was measured independently to be 11.35 mW using a quartz cuvette cell containing pure water. *I* is the laser power density (2 W/cm²), A_{808} is the absorbance of composite hydrogel at the excitation wavelength of 808 nm ($A_{808} = 9.58$). Note that the concentration of pBP in the tested hydrogel was set as 0.1 mg/mL, due to the absorbance of hydrogel with higher pBP concentration will exceed the measuring range of the spectrometer. Thus, only the *hS* remains unknown for calculating η .

In order to get the *hS*, a dimensionless driving force temperature, θ is introduced using the maximum system temperature (T_{max}) and a sample system time constant (τ_s):

$$hS = \frac{\sum mC_P}{\tau_s}$$
(2)
$$\tau_s = -\frac{t}{\ln^{10}(\theta)}$$
(3)
$$\theta = \frac{T_{surr} - T}{T_{surr} - T_{max}}$$
(4)

where *m* and C_p are the mass and specific heat capacity of the composite hydrogel. *t* is the time of cooling process, *T* is the real-time temperature of *t*. It is worth to note that the mass ratio of PVA in composite hydrogel was only 8% and the water was totally entrapped within the formed hydrogel, therefore, according to Wang *et al*'s study,² the specific heat capacity of the hydrogel can be approximate to pure water ($C_{H2O} = 4.2 \text{ J/g}$).

As shown in Figure 7(d), by applying the linear time data (t) from the cooling process versus

negative natural logarithm of driving force temperature (θ), τ_s is determined to be 187 s. Thus, according to Eq. (2), the *hS* is deduced to be 22.45 mW/°C. According to Eq. (1), the photothermal conversion efficiency (η) of PVA/pBP hydrogel is calculated to be 31.5%.

2. Supplementary Figures

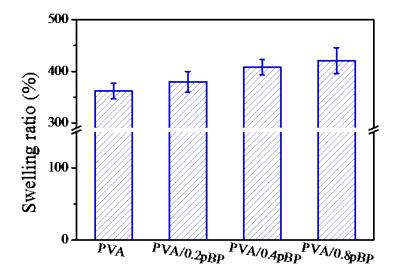


Figure S1. Swelling ratio of the PVA/pBP composite hydrogels.

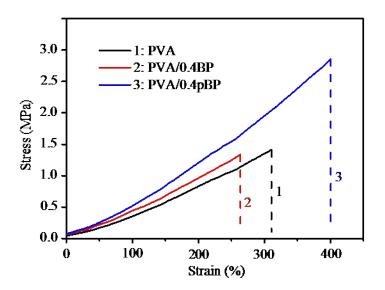


Figure S2. Stress-strain curves of PVA hydrogel, PVA/0.4BP hydrogel and PVA/0.4pBP hydrogel.

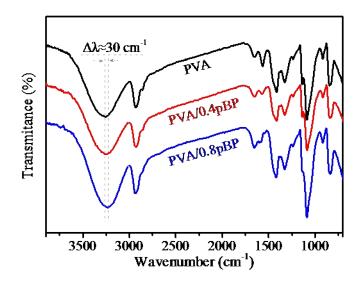


Figure S3. FTIR spectra of the PVA/pBP composite hydrogels.

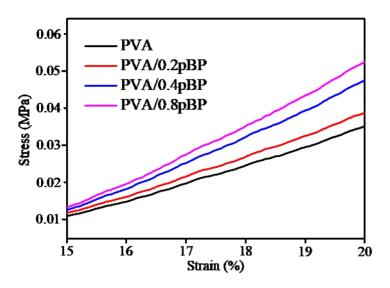


Figure S4. The clarified linear portion of the stress-strain curves of the composite hydrogels under compression.

References

- 1. D. K. Roper, W. Ahn and M. Hoepfner, *J Phys Chem C*, 2007, **111**, 3636-3641.
- 2. J. L. Zhao, J. L. Li, C. P. Zhu, F. Hu, H. Y. Wu, X. H. Man, Z. S. Li, C. Q. Ye, D. W. Zou and

S. G. Wang, Acs Appl Mater Inter, 2018, DOI: 10.1021/acsami.7b17608.