

## Supporting Information

### **Novel perylene probe-encapsulated metal-organic framework nanocomposites for ratiometric fluorescence detection of ATP**

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## EXPERIMENTAL SECTION

### Optimization of reaction time for ATP sensing

ATP was added to PDI@ZIF-8<sub>50</sub> dispersion in Tris-HCl buffer (5 mM, pH 7.4) and the resulted mixture (final sample volume: 200 μL) was incubated at 25 °C in a water bath for different time (0, 2, 5, 10, 20, 30, 40, 50 and 60 min, respectively). Then the fluorescence spectra were recorded. Final concentrations: PDI@ZIF-8<sub>50</sub>, 40 μg/mL; ATP, 500 μM.

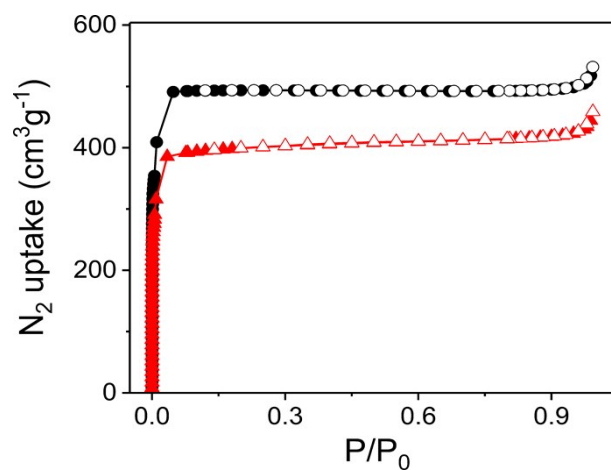
### Encapsulation efficiency ( $E_{\text{encapsulation}}$ ) of PDI in PDI@ZIF-8

$$E_{\text{encapsulation}} = \frac{A_{\text{PDI@ZIF-8}}}{A_{\text{PDI}}}$$

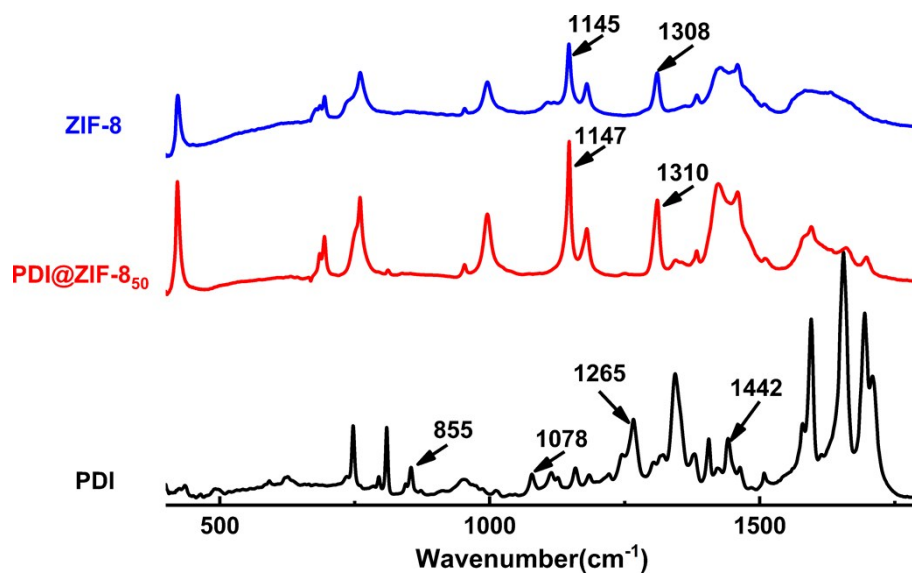
$A_{\text{PDI@ZIF-8}}$  is the absorbance of PDI probe at 500 nm which is released from PDI@ZIF-8 following the decomposition triggered by 7.5 mM ATP;  $A_{\text{PDI}}$  is the absorbance of PDI probe at 500 nm which is initially employed for the synthesis of PDI@ZIF-8.

Methods	System	Detection Limit	Linear range	Reference
Surface plasmon resonance	LSPR array chip	10 nM	0.01-100 $\mu$ M	S1
Electrochemical	Cascade enzymatic reactions	49 nM	0.05-0.4 $\mu$ M	S2
Fluorescence	Two conjugated polymers	2.5 $\mu$ M	0-180 $\mu$ M	S3
Fluorescence	FRET-based DNA nanoprism	30 $\mu$ M	0.03-2 mM	S4
Fluorescence	Oligonucleotide-templated Ag nanoclusters	33 nM	0.1-10 $\mu$ M	S5
Colorimetric	Stimuli-responsive DNA hydrogels	5.6 $\mu$ M	5-100 $\mu$ M	S6
Electrochemical	Electrochemical current rectification	114 nM	0-5 $\mu$ M	S7
Optomagnetic biosensor	Magnetic nanoparticle clustering	74 $\mu$ M	0.1-3 mM	S8
Fluorescence	Perylene probe encapsulated ZIF-8	10 $\mu$ M	10-175 $\mu$ M	This work

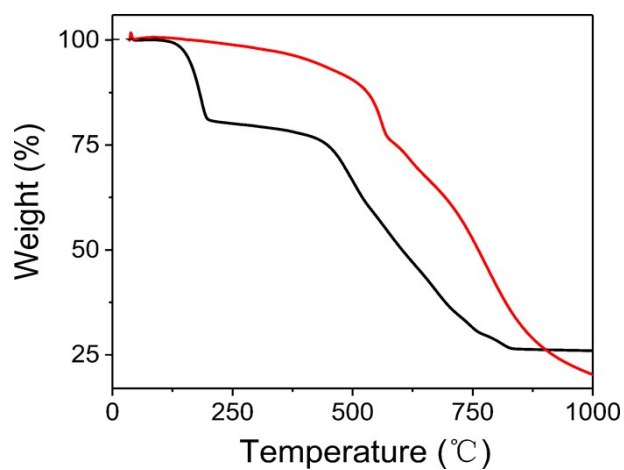
**Table S1.** The comparison between our method and some other reported methods



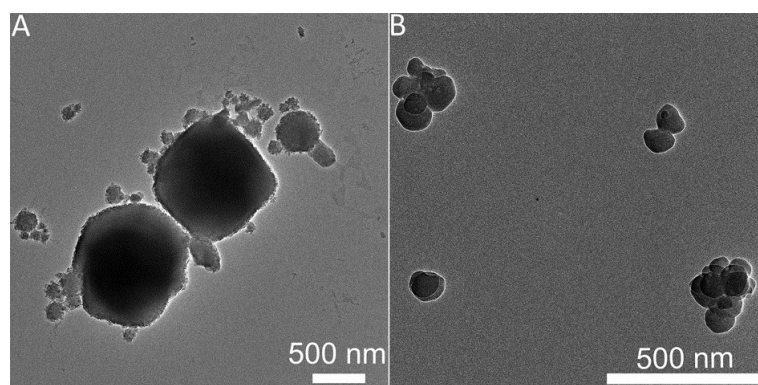
**Figure S1.** Nitrogen absorption isotherms of pure ZIF-8 nanocrystals (black) and PDI@ZIF-8<sub>50</sub> nanocomposites (red).



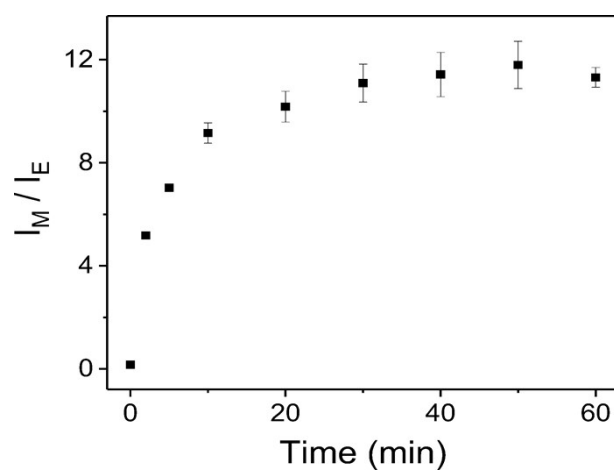
**Figure S2.** FT-IR spectra of pure ZIF-8 nanocrystals (blue), PDI@ZIF-8<sub>50</sub> nanocomposites (red) and PDI (black).



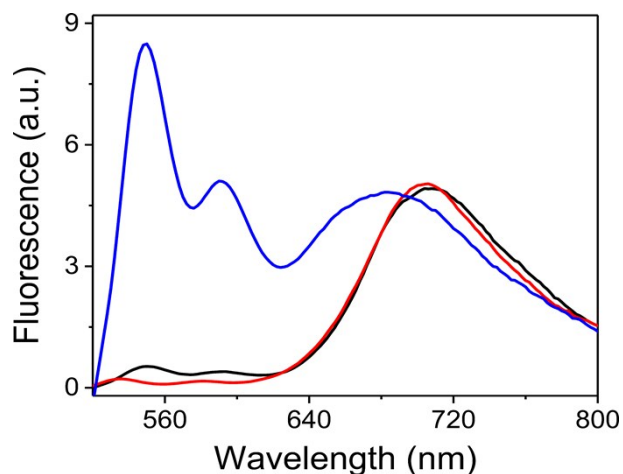
**Figure S3.** TGA curves of pure ZIF-8 nanocrystals (black) and PDI@ZIF-8 nanocomposites (red).



**Figure S4.** TEM images of PDI@ZIF-8<sub>25</sub> (A) and PDI@ZIF-8<sub>100</sub> (B) nanocomposites.



**Figure S5.** Changes in  $I_M/I_E$  value of PDI@ZIF-8<sub>50</sub> nanocomposites with the reaction time for ATP sensing.



**Figure S6.** Fluorescence emission spectra of PDI@ZIF-8<sub>50</sub> in buffers of different pH values: pH=3.3 (red), pH=7.4 (black) and pH=10.0 (blue).

## References

- S1. L. Xie, X. Yan and Y. Du, *Biosens. Bioelectron.*, 2014, **53**, 58-64.
- S2. J. K. Ahn, H. Y. Kim, K. S. Park and H. G. Park, *Anal. Chem.*, 2018, **90**, 11340-11343.
- S3. Q. Zhao, Z. Zhang and Y. Tang, *Chem. Commun.*, 2017, **53**, 9414-9417.
- S4. X. Zheng, R. Peng, X. Jiang, Y. Wang, S. Xu, G. Ke, T. Fu, Q. Liu, S. Huan and X. Zhang, *Anal. Chem.*, 2017, **89**, 10941-10947.
- S5. J. D. Lee, J. Cang, Y. C. Chen, W. Y. Chen, C. M. Ou and H. T. Chang, *Biosens. Bioelectron.*, 2014, **58**, 266-271.
- S6. M. Oishi and K. Nakatani, *Small*, 2019, **15**, e1900490.
- S7. L. Feng, A. Sivanesan, Z. Lyu, A. Offenhausser and D. Mayer, *Biosens. Bioelectron.*, 2015, **66**, 62-68.
- S8. J. Yang, M. Donolato, A. Pinto, F. G. Bosco, E. T. Hwu, C. H. Chen, T. S. Alstrom, G. H. Lee, T. Schafer, P. Vavassori, A. Boisen, Q. Lin and M. F.

Hansen, *Biosens. Bioelectron.*, 2016, **75**, 396-403.