

Supporting Information

Surface-enhancement Raman scattering of all inorganic perovskite quantum dots CsPbBr₃ encapsulated in Metal-organic framework ZIF-8

Mingyang Xin ^a, Yuzhou Fu ^a, Yue Zhou ^a, Junhe Han^a, Yanli Mao^a, Mengjia Li ^b,
Junhui Liu ^{*a}, Mingju Huang ^{*a}

^aKey Laboratory of International Joint Research Laboratory of New Energy

Materials and Devices of Henan Province, School of Physics and Electronics, Henan

University, Kaifeng 475004, China

^bSchool of Materials Science and Engineering, Zhengzhou University,

Zhengzhou, 450001, China

* Corresponding author.

E-mail addresses: liujh@henu.edu.cn (Junhui Liu), hmingju@163.com (Mingju Huang).

Materials

Silver nitrate (AgNO₃, AR, 99.8%), polyvinylpyrrolidone (PVP, K30), sodium citrate (AR, 99.0%), Lead (II) bromide (PbBr₂, 99.999%), cesium bromide (CsBr, 99.999%), 6-Mercaptopurine (6-MP), N, N-Dimethylformamide (DMF), 4-Mercaptopyridine (4-MPY), Methanol, Ethanol, Cyclohexane and zinc nitrate hexahydrate (Zn(NO₃)₂·6H₂O, 99.999%) were obtained from Aladdin Industrial Corporation. 2-Methylimidazole (2-MIM) was purchased from Spectrochem. Toluene is redistilled prior to use and other solvents are treated with 4A molecular sieves.

Preparation of calcium titanium composite assembled substrates.

Clean 0.5cm x 1cm silicon with an ultrasonic cleaner using deionized water, ethanol, acetone, chloroform, acetone, ethanol, and deionized water in turn. Rinse off residual organic solvents with deionized water. Boiling by immersing wafers in a mixture of 30% H₂O₂ and 98% H₂SO₄ with a volume ratio of 3:7 solution. After cooling, rinse the wafer repeatedly with deionized water. Eventually, the wafer surface is covered with hydroxyl groups.

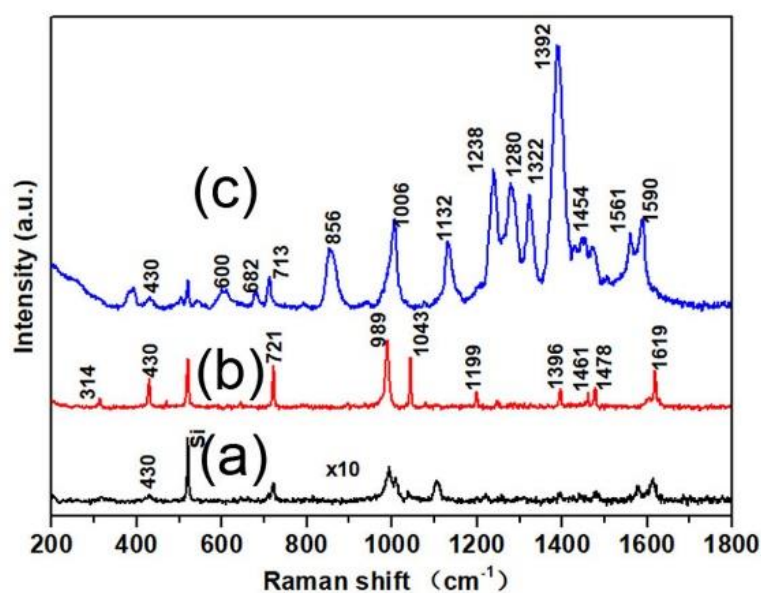


Fig.S1 (a) Raman diagram of 6-MP. (b) SERS diagram of 6-MP adsorbed on the composites surface. (c) SERS diagram of 6-MP adsorbed on an Ag surface.

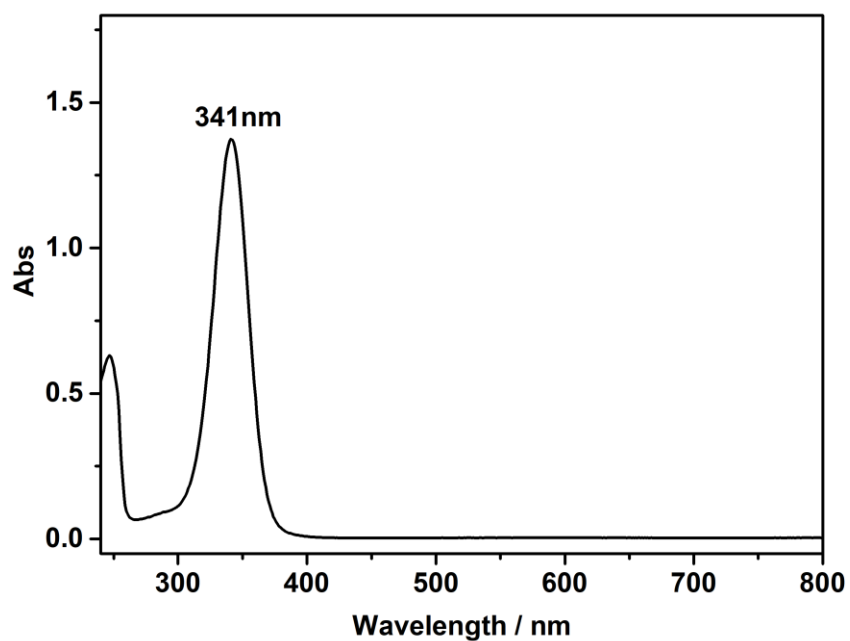


Fig. S2 UV-Vis spectra of 4-MPY.

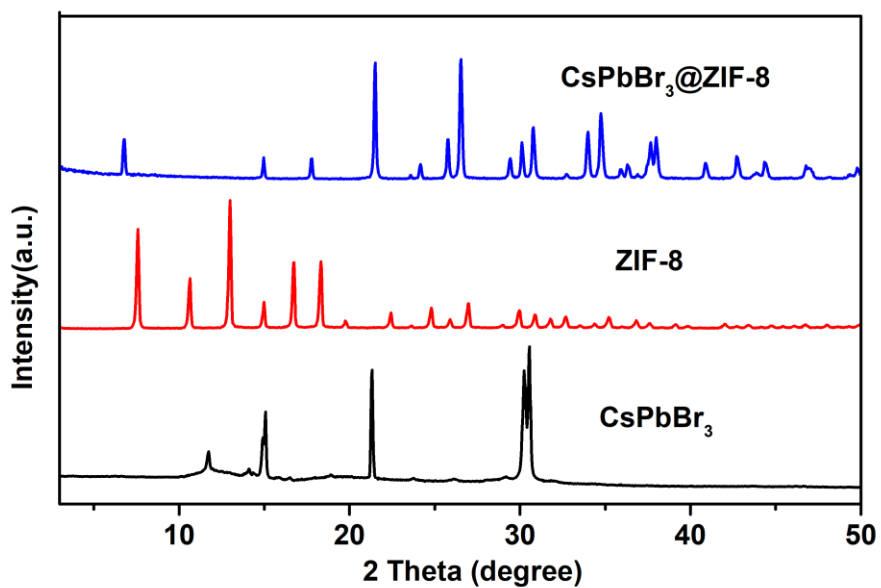


Fig. S3 Comparison of PXRD patterns of CsPbBr₃, ZIF-8, CsPbBr₃@ZIF-8.

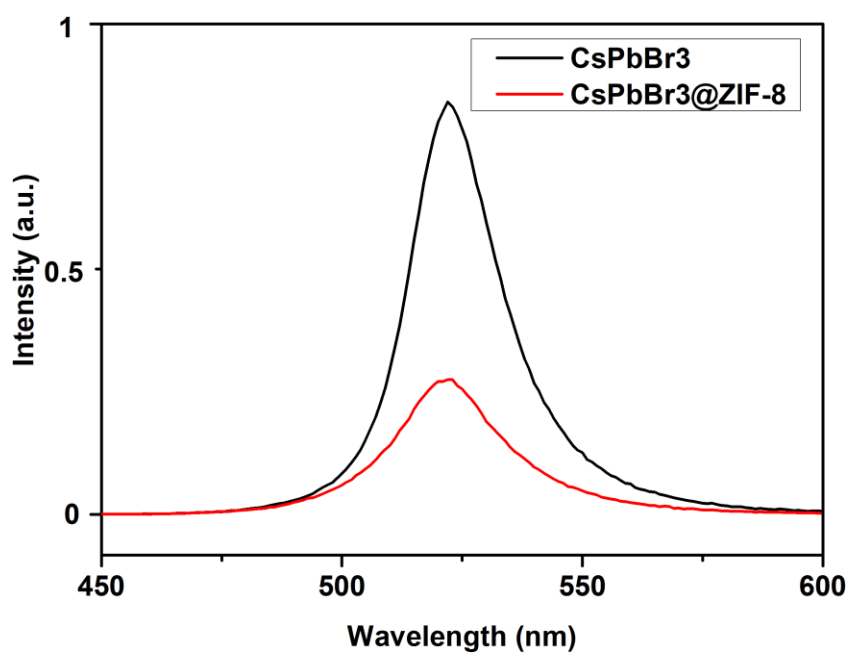


Fig. S4 Steady-state PL spectra.

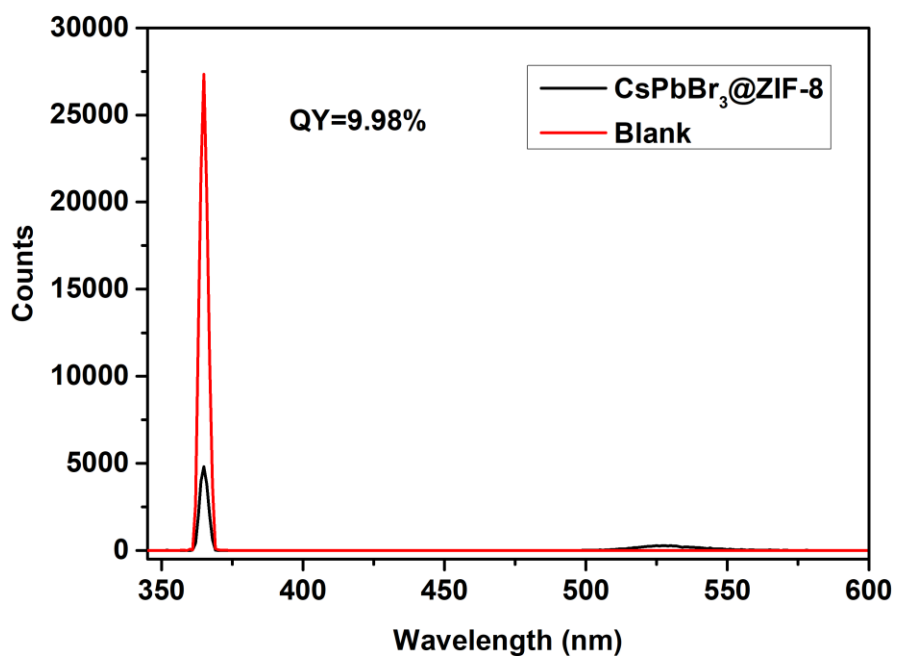


Fig. S5 PLQY of CsPbBr₃@ZIF-8.

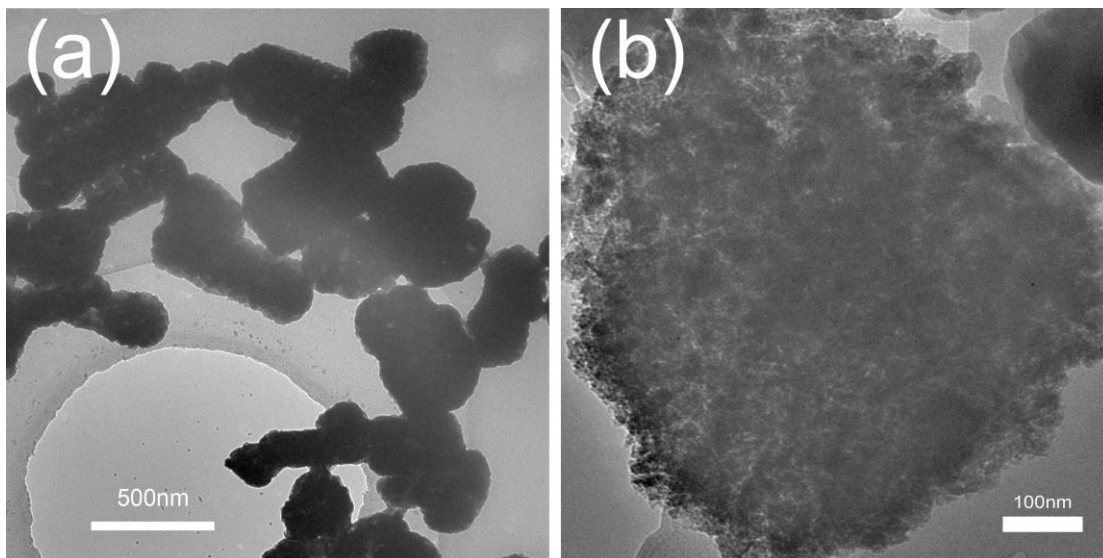


Fig. S6 TEM pictures of composite material CsPbBr₃@ZIF-8.

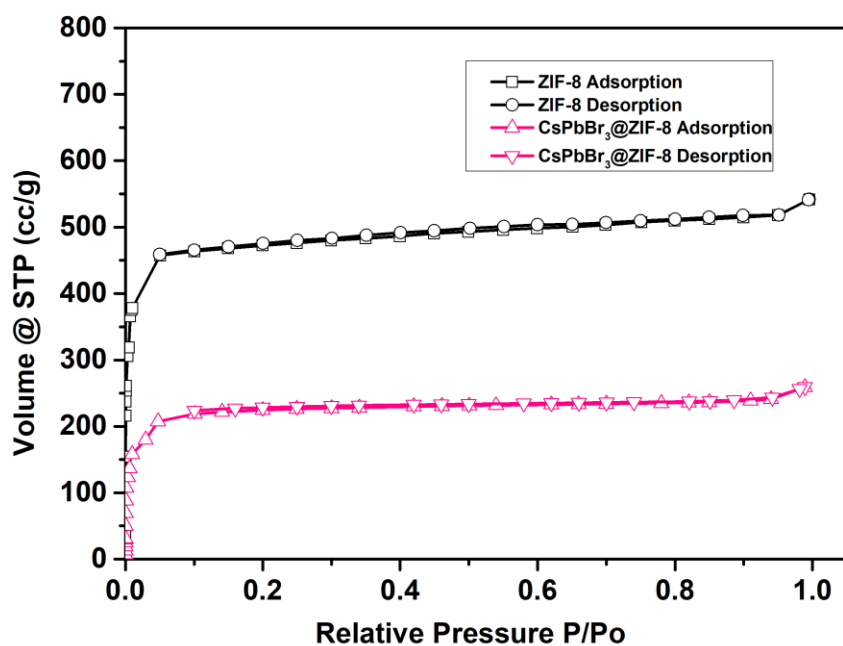


Fig. S7 N₂ gas adsorption at 77 K for ZIF-8 and CsPbBr₃@ZIF-8 composite. The gas uptake amount for composite is relatively low due to formation of CsPbBr₃ NCs inside ZIF-8 cavity.

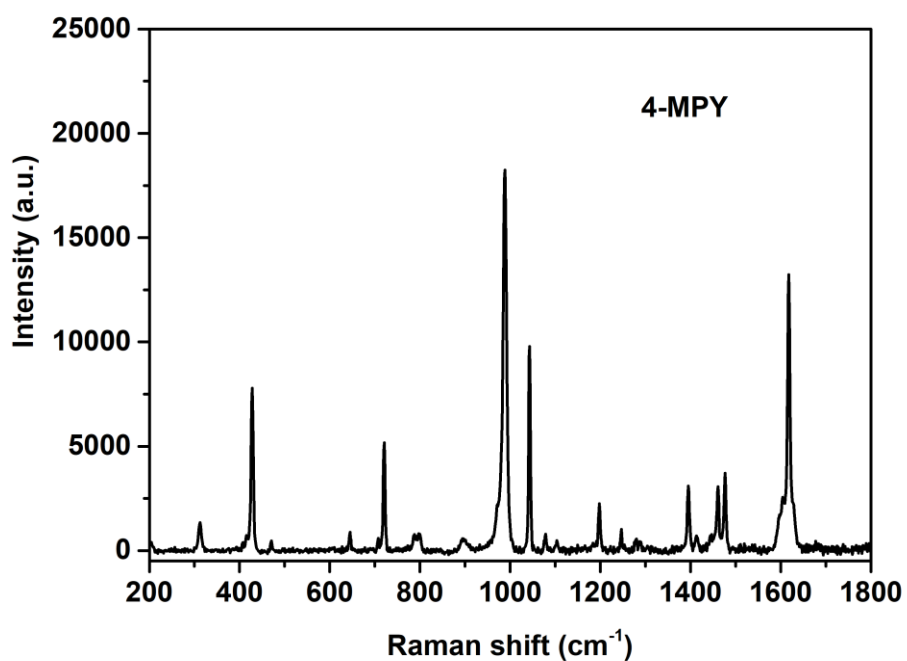


Fig. S8 Normal Raman spectrum of 4-MPY (0.3M).

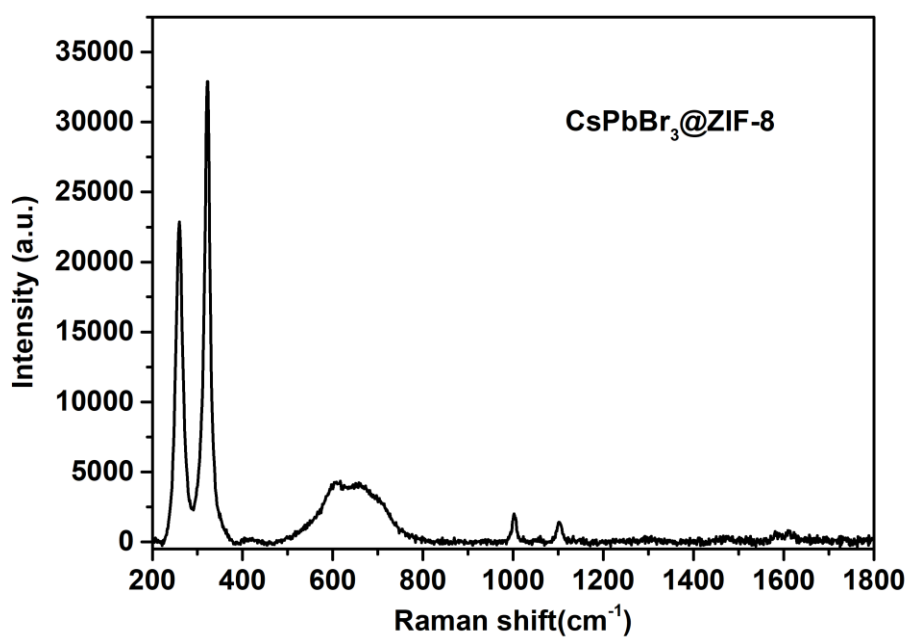


Fig. S9 Normal Raman spectrum of CsPbBr₃@ZIF-8.

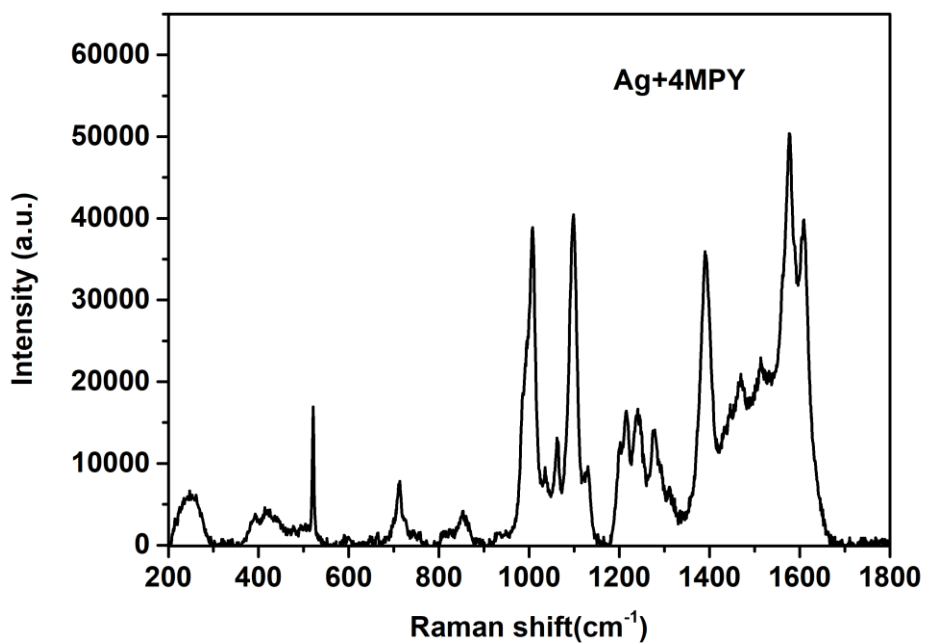


Fig. S10 SERS spectra of 4-MPY adsorbed on Ag film.

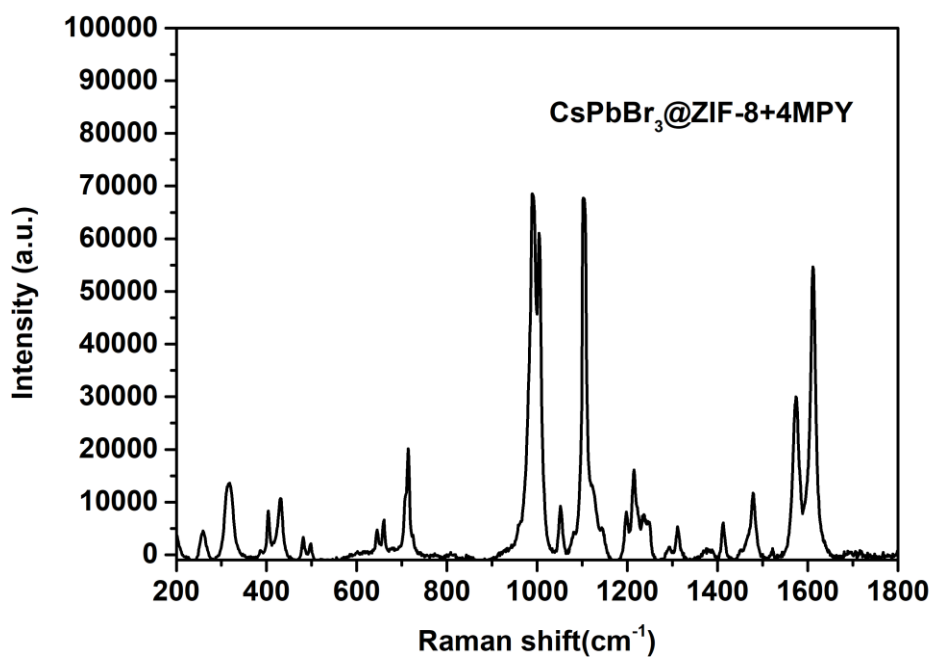


Fig. S11 SERS spectra of 4-MPY adsorbed on CsPbBr₃@ZIF-8.

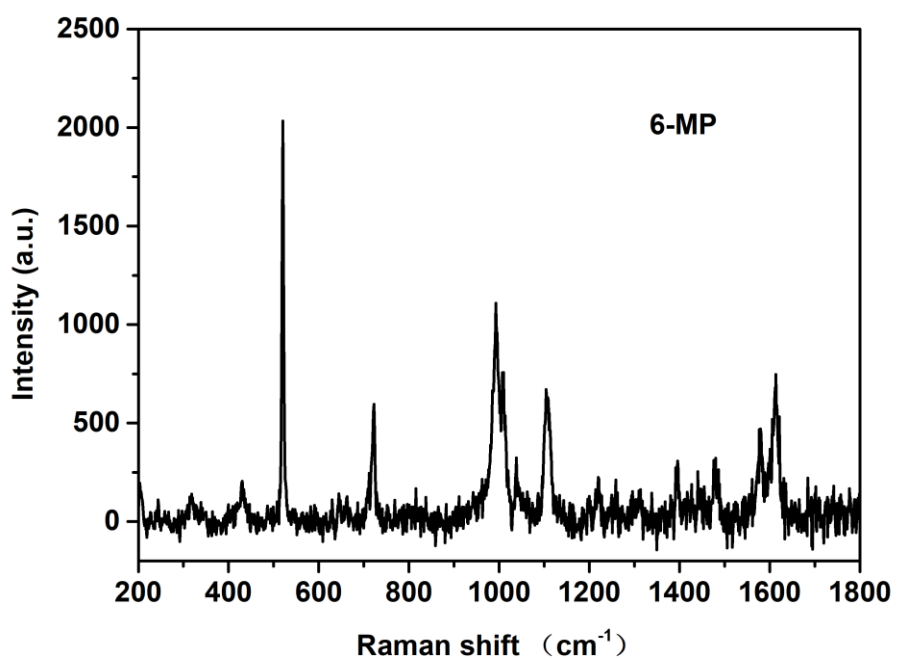


Fig. S12 Raman diagram of 6-MP (0.3M).

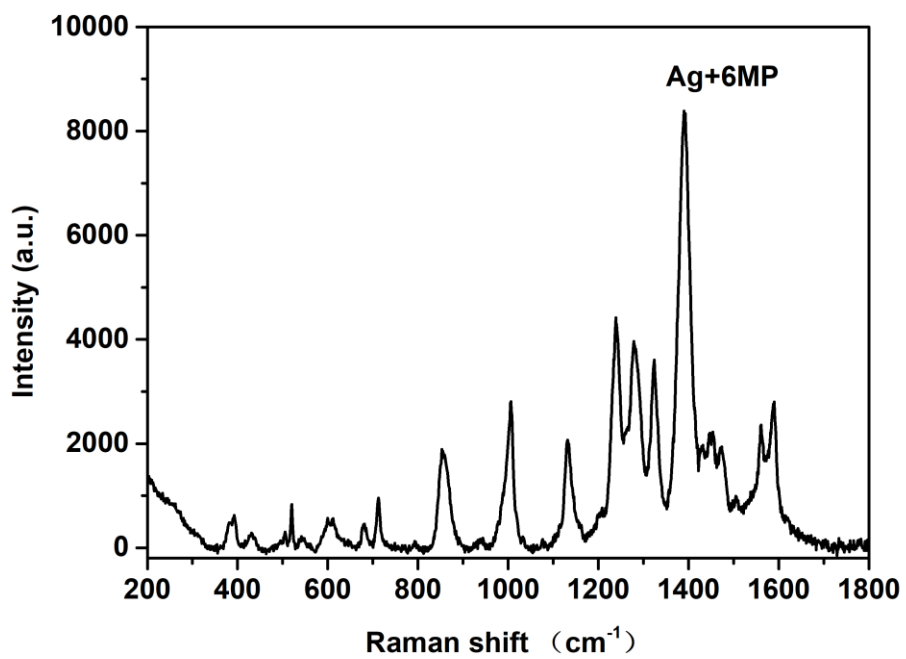


Fig. S13 SERS diagram of 6-MP adsorbed on an Ag surface.

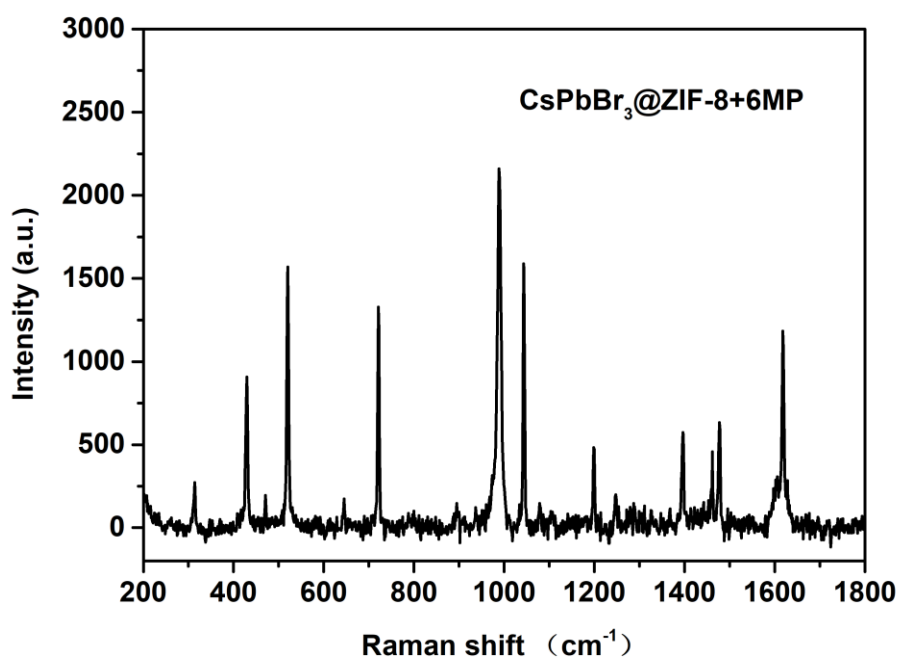


Fig. S14 SERS diagram of 6-MP adsorbed on the composites surface.

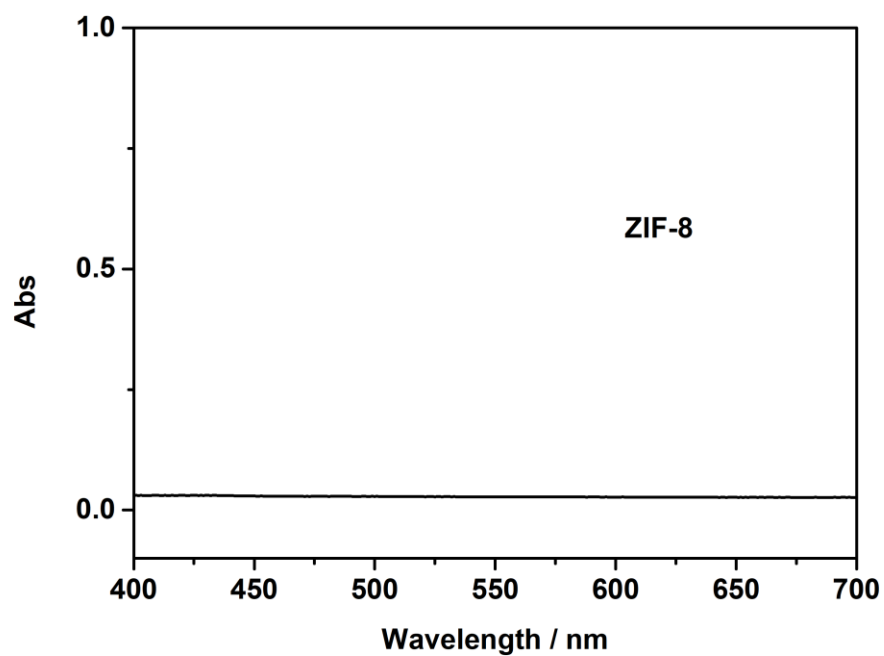


Fig. S15 UV-Vis spectra of ZIF-8.

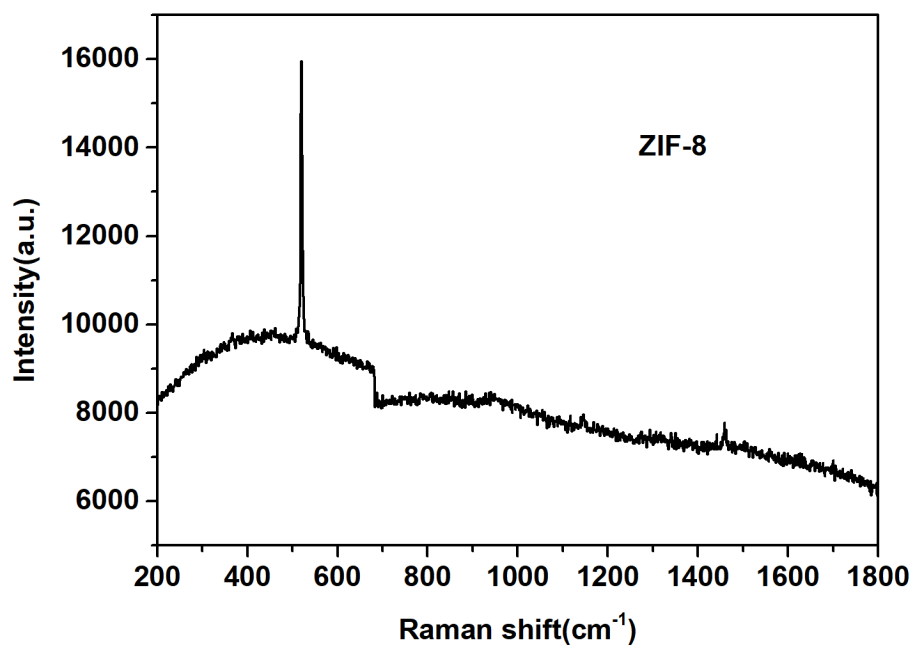


Fig. S16 Normal Raman spectrum of ZIF-8.

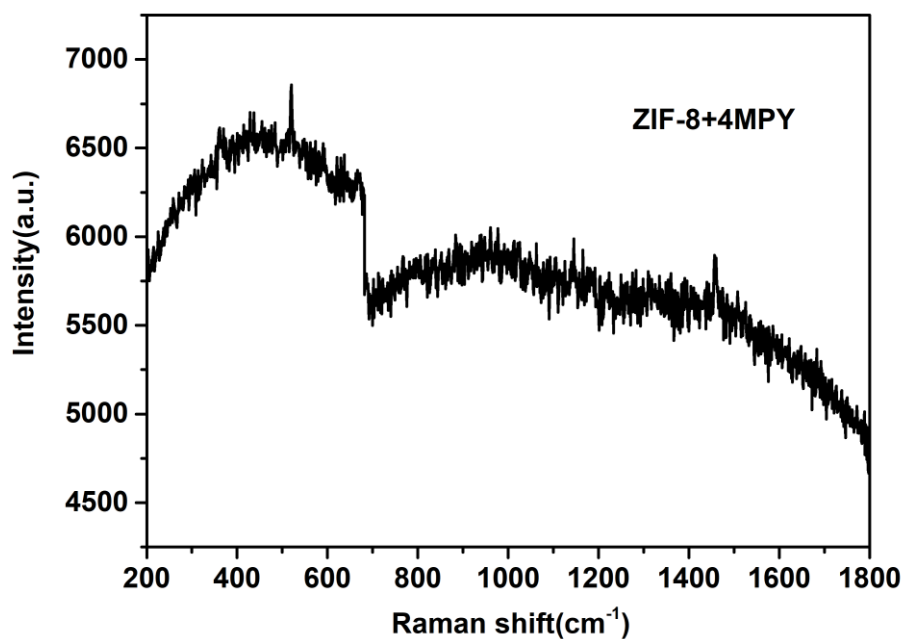


Fig. S17 SERS diagram of 4-MPY adsorbed on the ZIF-8 surface.

Table S1. Raman/SERS shifts (cm^{-1}) and band assignments of 4-Mpy on the Ag and $\text{CsPbBr}_3@ZIF-8$ substrates.

4MPY	Ag+4MPY	$\text{CsPbBr}_3@zif8+4MPY$	assignments
428	426	430	7a1 δ (C-S)/ γ (CCC)
720	711	713	6a1 β (C-C)/ ν (C-S)
988	1008	988	a1 ring breathing
1043	1061	1051	18a1 ring breathing β (CH)
1106	1098	1106	12a1 ring breathing / ν (C-S)
1198	1202	1197	9a1 β (CH)/ δ (NH)
1246	1221	1236	9a1 β (CH)
1395	1390	1412	14b2 ν (C=C)
1476	1469	1479	19a1 ν (C=C/C=N)
1604	1577	1573	8b2 ν (C=C)
1617	1609	1611	8a1 ν (C=C)

Assignments from Refs^{1, 2, 3}

[1] F.R. Dollish, F.F. Bentley, W.G. Fateley, *microelectronics journal*, 1974, 37(5):395-403.

[2] J.H.S. Green, W. Kynaston, H.M. Paisley, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 1963, 19(2):549-564.

[3] T.H. Joo, M.S. Kim, K. Kim, *Journal of Molecular Structure*, 1987, 160(1-2):81-89.