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

Supplementary Information

Efficient Encapsulation of $CsPbBr_3$ and Au nanocrystals in Mesoporous Metal–Organic Frameworks Towards Synergetic Photocatalytic CO_2 Reduction

Jia-Nan Huang, Yu-Jie Dong, Hai-Bing Zhao, Hong-Yan Chen, Dai-Bin Kuang and Cheng-Yong Su**

MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, Lehn Institute of Functional Materials, School of Chemistry, Sun Yat-sen University, Guangzhou 510006, P. R. China.

E-mail: chenhy33@mail.sysu.edu.cn; cesscy@mail.sysu.edu.cn

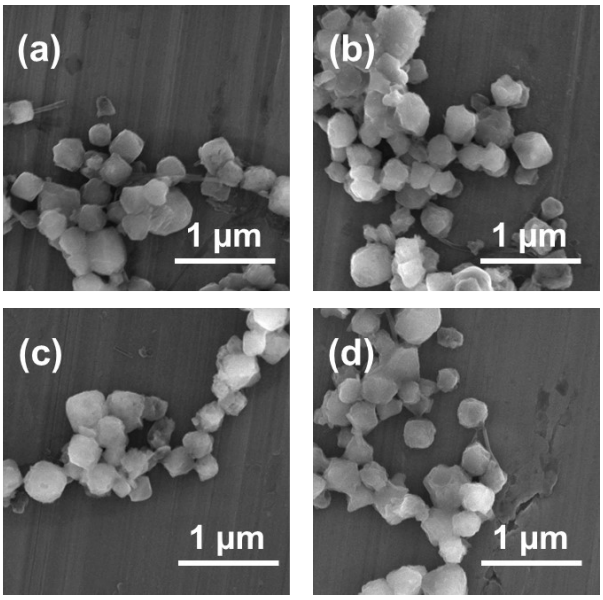

Figure S1. SEM image of (a) PCN-333(Al), (b) Au/PCN-333(Al), (c) $CsPbBr_3$/PCN-333(Al) and (d) $CsPbBr_3$/Au/PCN-333(Al).

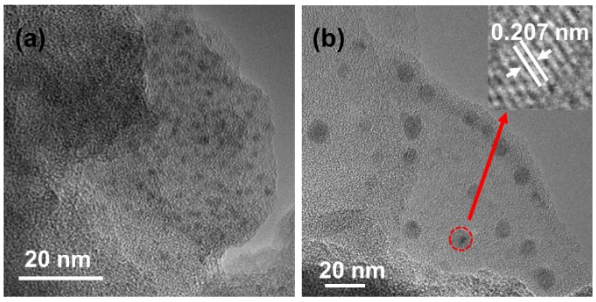

Figure S2. (a) TEM image of Au/PCN-333(Al). (b) TEM image of $CsPbBr_3$/PCN-333(Al).

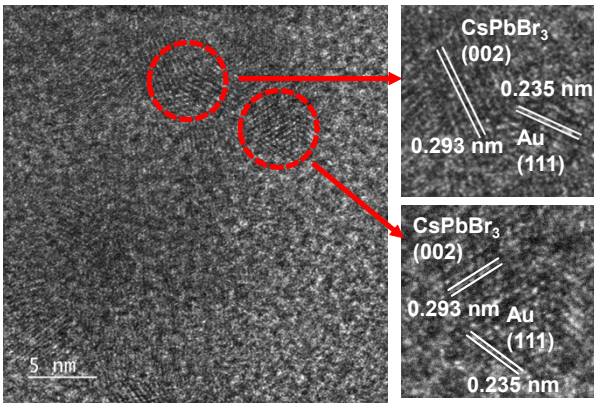

Figure S3. High resolution ultrathin section TEM image of $CsPbBr_3$/Au/PCN-333(Al).

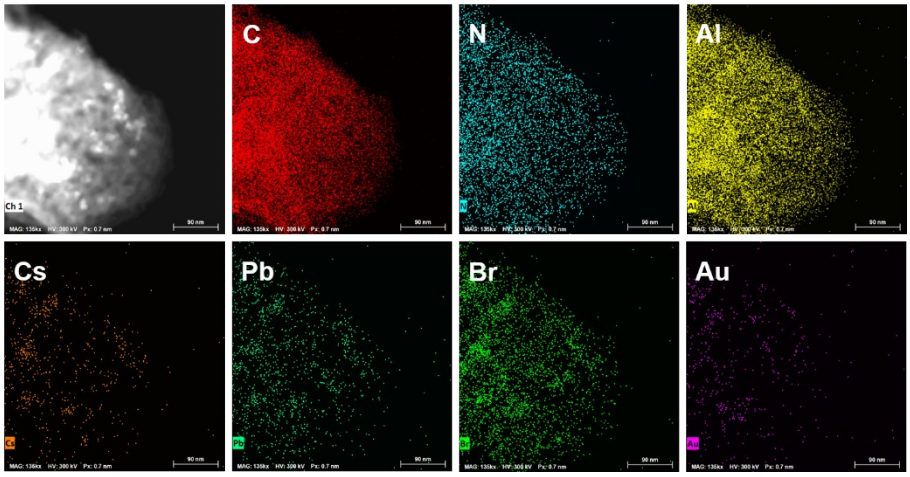

Figure S4. The elemental mapping images of $CsPbBr_3$/Au/PCN-333(Al).

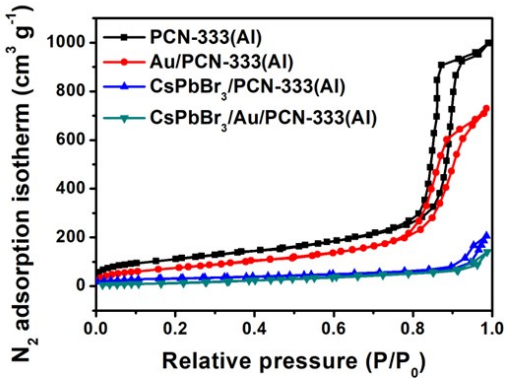

Figure S5. N_2 sorption isotherms of different samples at 77 K and 1 atm.

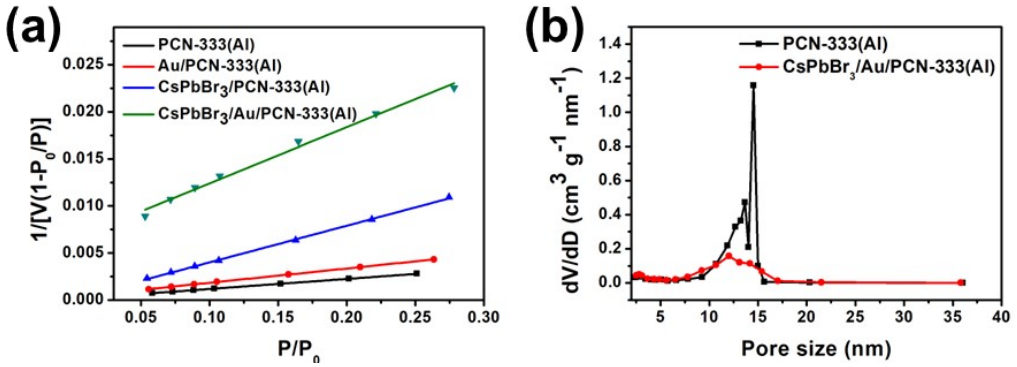

Figure S6. (a) The linear BET equation fitting results of different samples. (b) Comparison of DFT pore size distributions before and after encapsulating the Au and perovskite (obtained from N_2 sorption isotherm at 77 K and 1 atm).

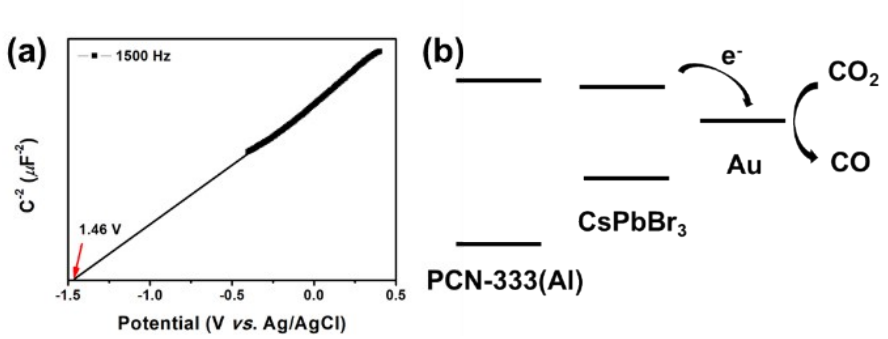

Figure S7. (a) Mott-Schottky plot of PCN-333(Al). (b) Schematic diagram of the relative energy band position of PCN-333(Al), $CsPbBr_3$ and Au.

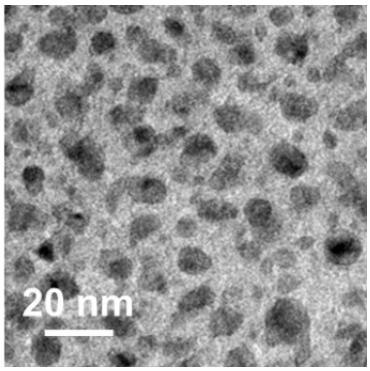

Figure S8. TEM image of $CsPbBr_3$ nanocrystals.

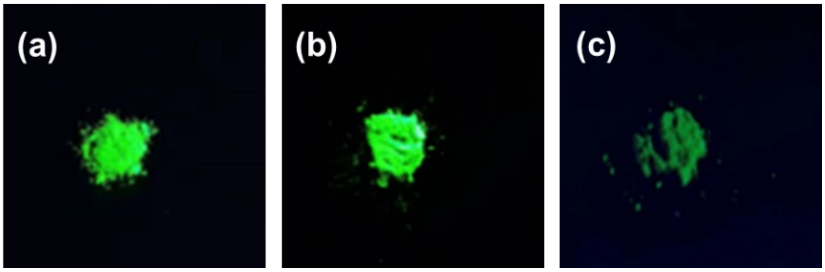

Figure S9. Photographs of samples excited at 365 nm: (a) $CsPbBr_3$ NCs, (b) $CsPbBr_3$/PCN-333(Al); (c) $CsPbBr_3$/Au/ PCN-333(Al).

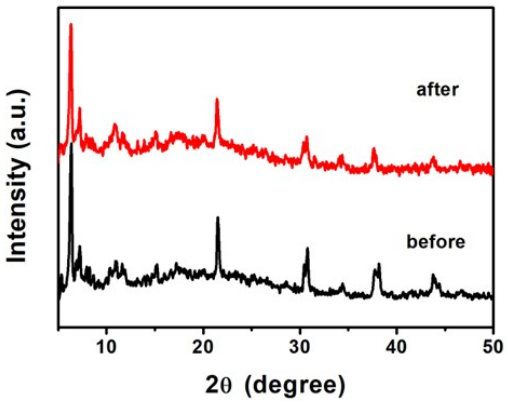

Figure S10. XRD pattern of $CsPbBr_3$/Au/PCN-333(Al) after 5 photocatalytic cycles.

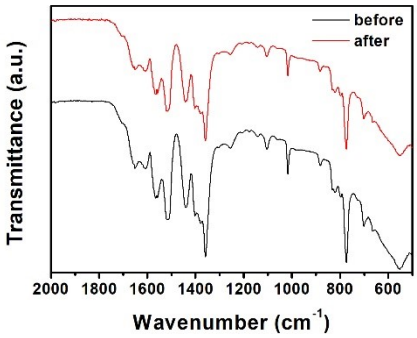

Figure S11. FTIR spectra of $CsPbBr_3$/Au/PCN-333(Al) before and after 5 photocatalytic cycles.

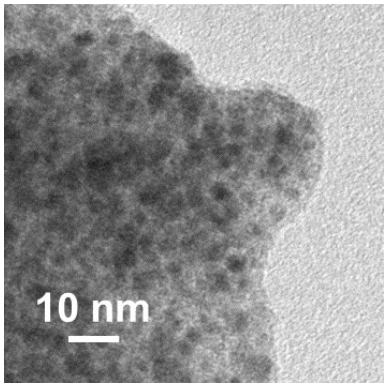

Figure S12. TEM image of $CsPbBr_3$/Au/ PCN-333(Al) after 5 photocatalytic cycles.

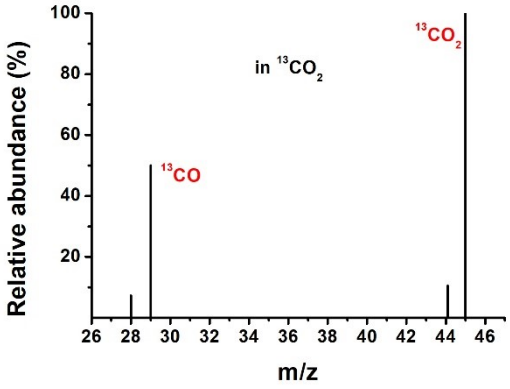

Figure S13. GC-MS spectra of isotope labeling catalytic products within $^{13}CO_2$ atmosphere.

Table S1. The content of each component in the composite sample ICP-MS

Sample	Au/wt%	$CsPbBr_3$/wt%
Au/PCN-333(Al)	5.8	-
$CsPbBr_3$/PCN-333(Al)	-	44.8
$CsPbBr_3$/Au/PCN-333(Al)	3.1	43.2

Table S2. Fitted PL decay parameters of $CsPbBr_3$, $CsPbBr_3$/PCN-333(Al) and $CsPbBr_3$/Au/PCN-333(Al).

Sample	τ_1/ns	A_1/%	τ_2/ns	A_2/%	$\tau_{average}$/ns
$CsPbBr_3$ NCs	6.63	44.38	69.97	55.62	41.86
$CsPbBr_3$/PCN-333(Al)	6.15	44.48	52.61	55.52	31.94
$CsPbBr_3$/Au/PCN-333(Al)	0.44	65.74	16.06	34.26	5.79

Table S3. Summary of photocatalytic performances of different catalysts after 3 h of reaction.

	Condition	$Yield_{CO}$ /μmol g^{-1}	$Yield_{CH_4}$ /μmol g^{-1}	$R_{electron}$[a] /μmol g^{-1} h^{-1}
No catalyst	CO_2	-	-	-
No light	CO_2	-	-	-
PCN-333(Al)	CO_2	-	-	-
Au/PCN-333(Al)	CO_2	-	-	-
$CsPbBr_3$ NCs	CO_2	7.41	2.22	10.83
$CsPbBr_3$/PCN-333(Al)	CO_2	28.65	6.48	36.38
$CsPbBr_3$/Au/PCN-333(Al)-low $CsPbBr_3$ loading	CO_2	101.85	-	67.89
$CsPbBr_3$/Au/PCN-333(Al)	CO_2	186.15	-	124.10
	N_2	8.49	0.17	6.12

[a] $R_{electron} = [2Yield_{CO}+8Yield_{CH_4}]/Time$