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

Supporting Information for

Construction of a multi-interfacial-electron transfer scheme for efficient CO_2 photoreduction: A case study using $CdIn_2S_4$ micro flower spheres modified with Au nanoparticles and reduced graphene oxide

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1. DFT analysis

The present first principle DFT calculations are performed with the projector augmented wave (PAW) method [1-2]. The exchange-functional is treated using the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) [3] functional. The cut-off energy of the plane-wave basis is set at 400 eV for optimize calculations of atoms and cell optimization. The vacuum spacing in a direction perpendicular to the plane of the catalyst is at least 10 Å. The Brillouin zone integration is performed using 3×3×1 Monkhorst-Pack k-point sampling for a primitive cell [4]. The self-consistent calculations apply a convergence energy threshold of 10^{-5} eV. The equilibrium lattice constants are optimized with maximum stress on each atom within 0.05 eV/Å. The Hubbard U (DFT+U) corrections for 3d transition metal by setting according to the literature [5]. Finally, the adsorption eneries (Eads) can be calculated by: Eads=$E_{surface+A}$-($E_{surface}$+E_A), where $E_{surface+A}$ is the energy of systems with CO_2 molecular adsorbed, Esurface is the energy of surface stcructure, and the EA is the energy of CO_2 molecular.

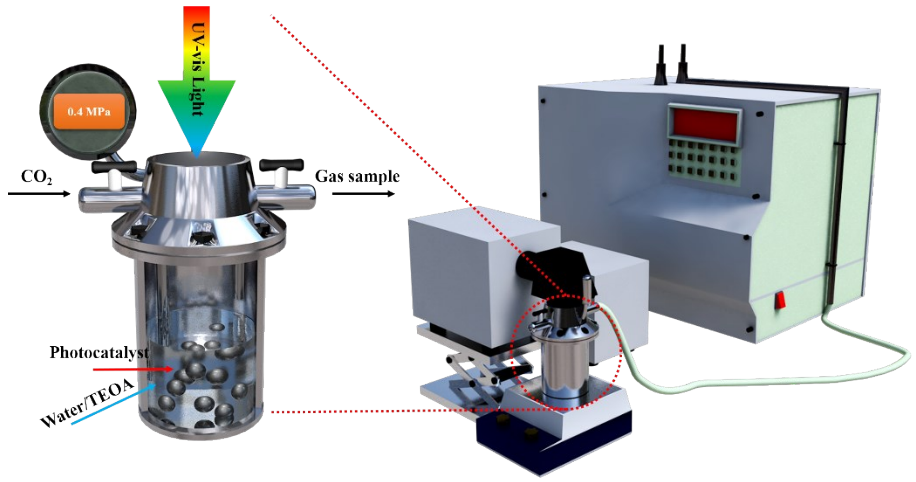

Fig. S1. The specific photocatalytic CO_2 reduction system.

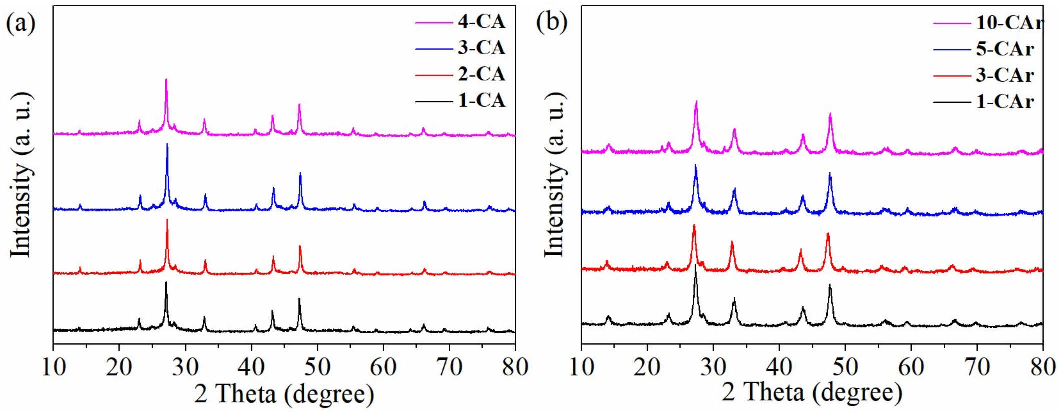

Fig. S2. XRD patterns of prepared binary and ternary composite photocatalysts.

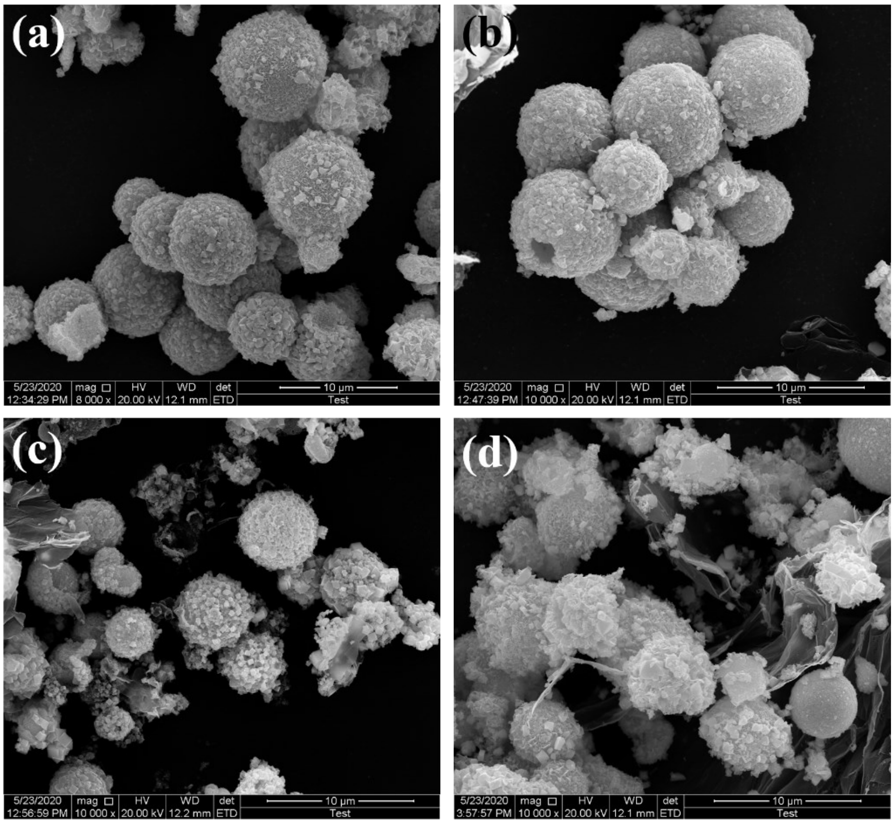

Fig. S3. SEM images of 1-CAr, 3-CAr, 5-CAr and 10-CAr.

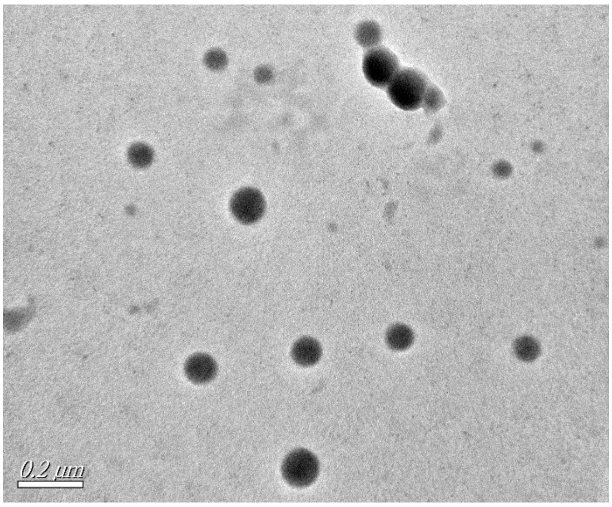

Fig. S4. TEM image of pure Au NPs.

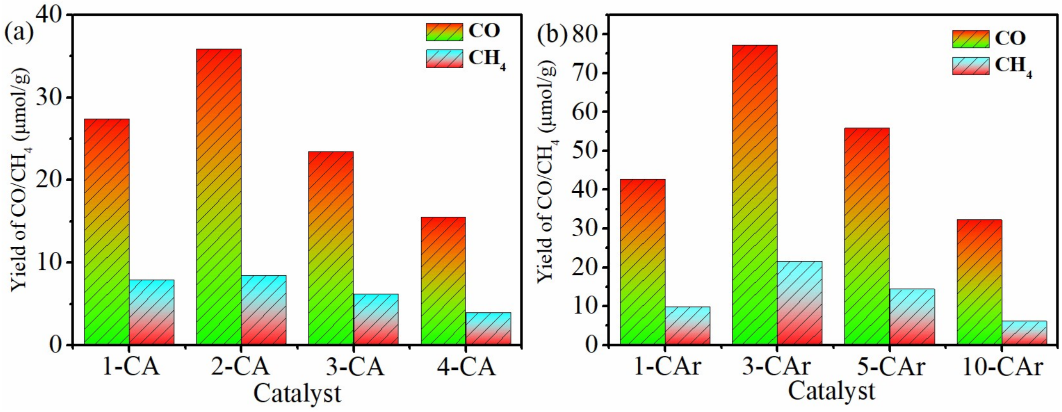

Fig. S5. The yields of CO and CH_4 in the photocatalytic CO_2 reduction process over all binary and ternary composite photocatalysts.

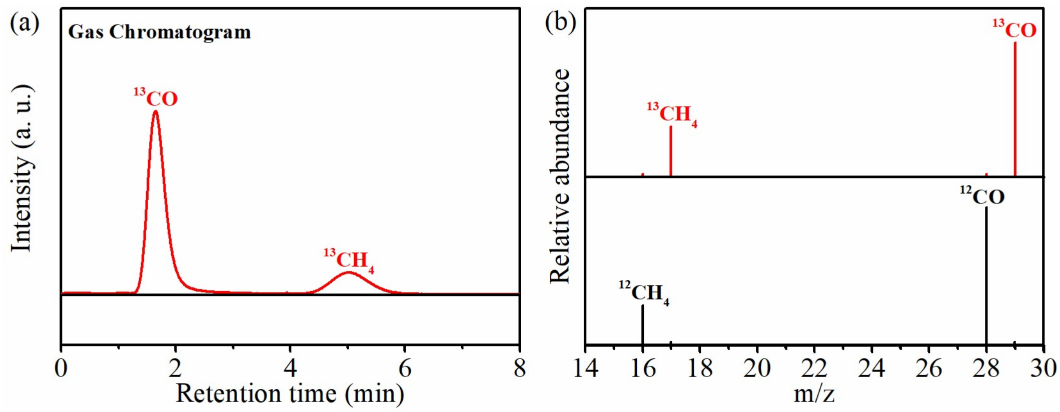

Fig. S6. Gas chromatography-mass spectrometry (GC-MS) results of CO and CH_4 produced by 3-CAr.

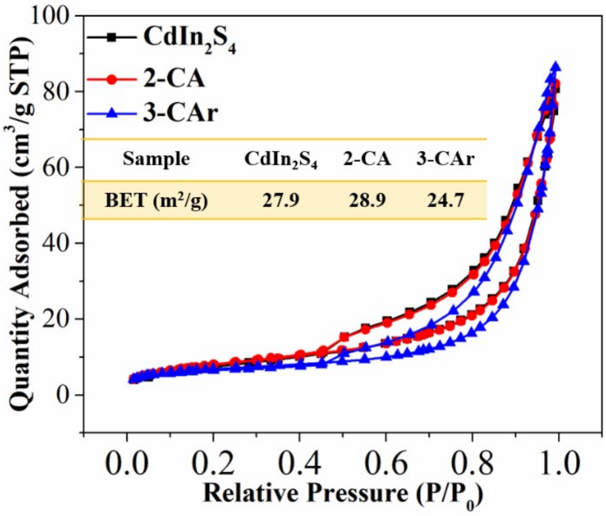

Fig. S7. N_2 adsorption-desorption isotherms of pure $CdIn_2S_4$, 2-CA and 3-CAr.

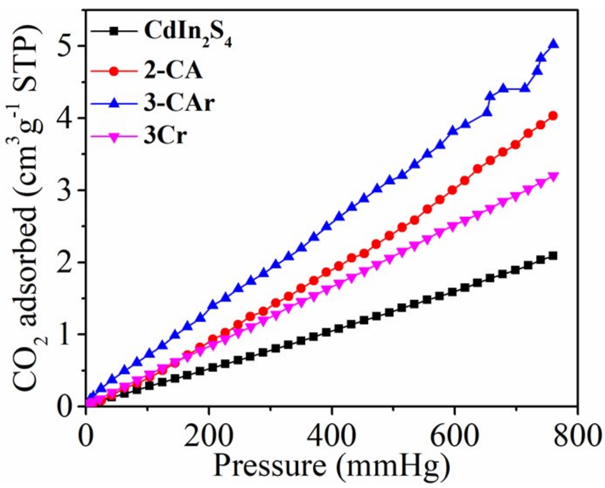

Fig. S8. CO_2 adsorption ability of pure $CdIn_2S_4$, 2-CA, 3-CAr and 3-Cr.

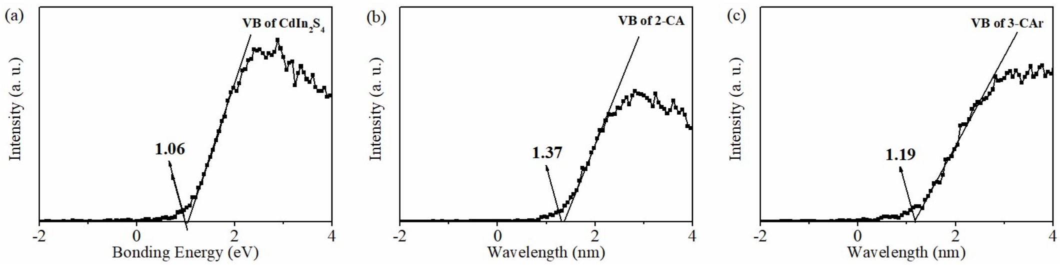

Fig. S9. The VB of pure $CdIn_2S_4$, 2-CA and 3-CAr.

References

[1] J. P. Perdew, K. Burke, M. Ernzerhof, Generalized Gradient Approximation Made Simple, Phys. Rev. Lett., 77 (1996) 3865.

[2] G. Kresse, D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method， Phys. Rev. B 59 (1999) 1758.

[3] J.P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Phy. Rev. Lett. 77 (1996) 3865.

[4] D.J. Chadi, Special points for Brillouin-zone integrations, Phys. Rev. B 16 (1977) 5188-5192.

[5] L. Gong, D. Zhang, C.Y. Lin, Y. Zhu, Y. Shen, J. Zhang, X. Han, L. Zhang, Z. Xia, Catalytic Mechanisms and Design Principles for Single-Atom Catalysts in Highly Efficient CO_2 Conversion, Advanced Energy Materials, 2019, 9, 1902625.