Supporting Information

Photocatalytic Conversion of 5-Hydroxymethylfurfural using Mixed Halide Perovskite $MAPbBr_xCl_{3-x}$ Quantum Dots

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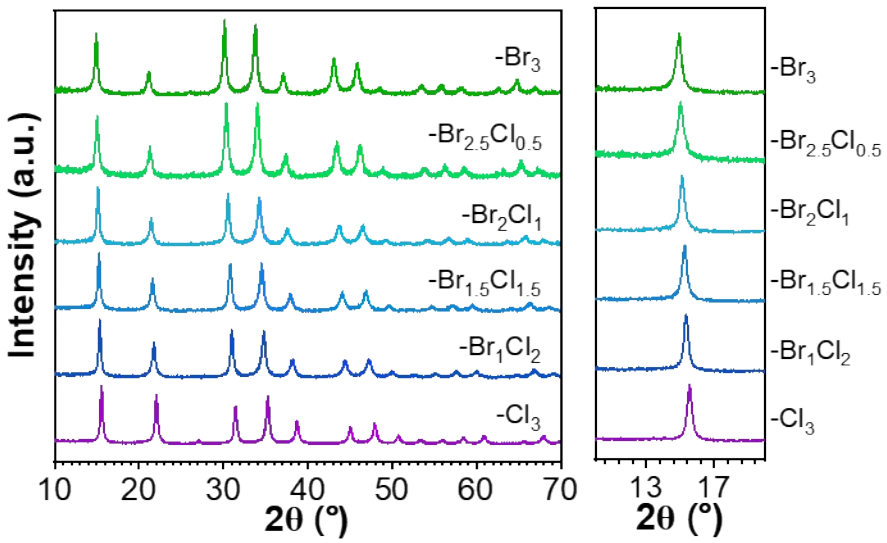

Figure S1. Enlarged XRD pattern corresponding to (001) plane of perovskite QDs samples.

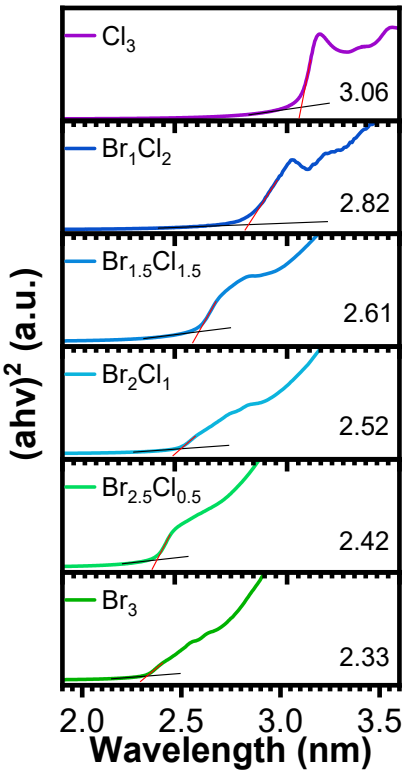

Figure S2. Method of band gap energy (Eg) determination from the Tauc plot for perovskite QDs samples.

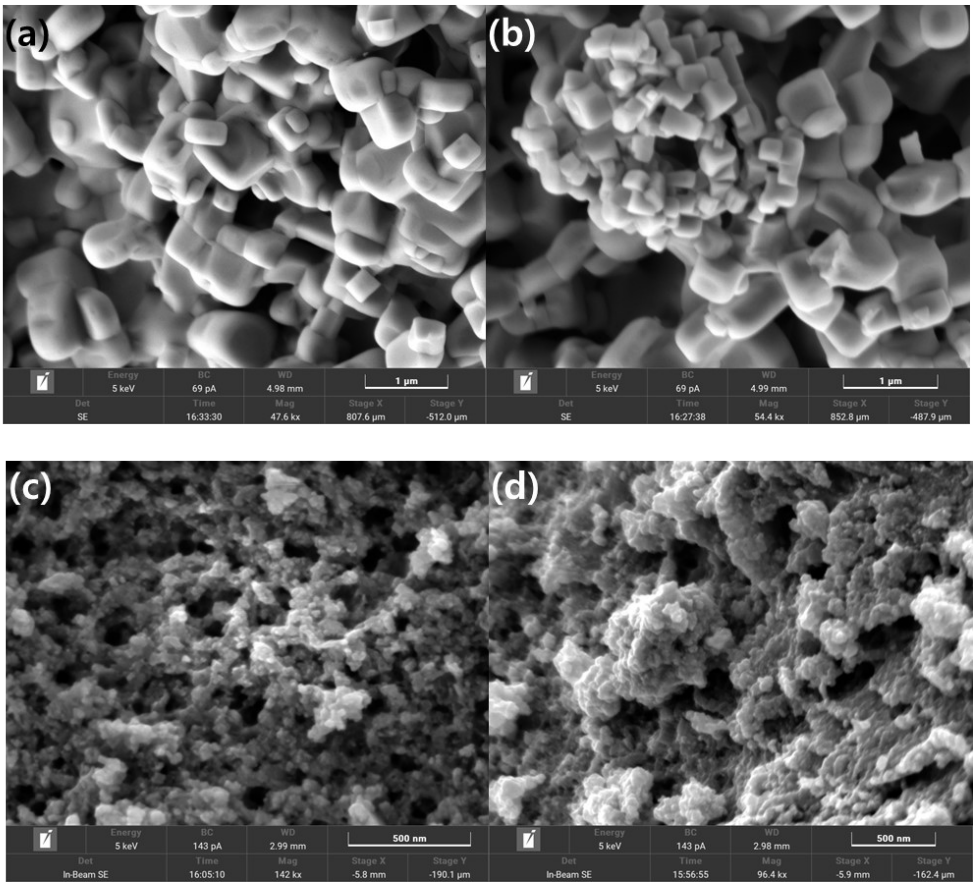

Figure S3. FE-SEM images of (a, b) $MAPbBr_2Cl_1$ bulk size materials and (c, d) $MAPbBr_2Cl_1$ QDs.

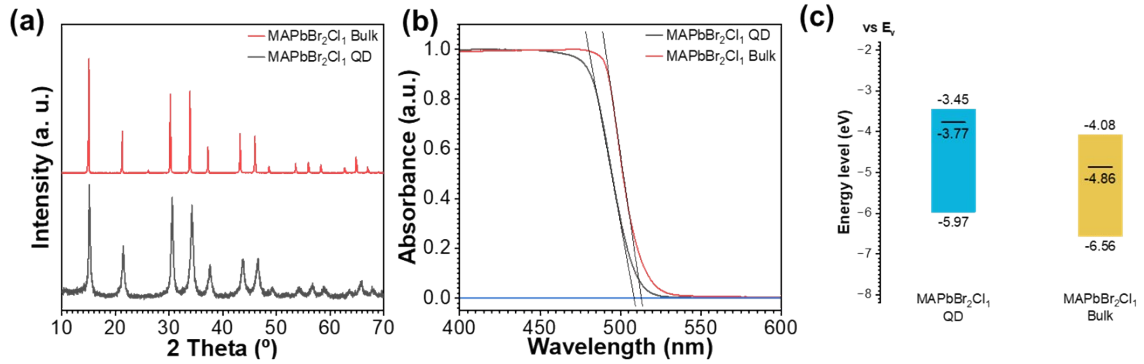

Figure S4. (a) XRD pattern, (b) optical band gap energy and (c) band edge position of $MAPbBr_2Cl_1$ bulk size materials and $MAPbBr_2Cl_1$ QDs.

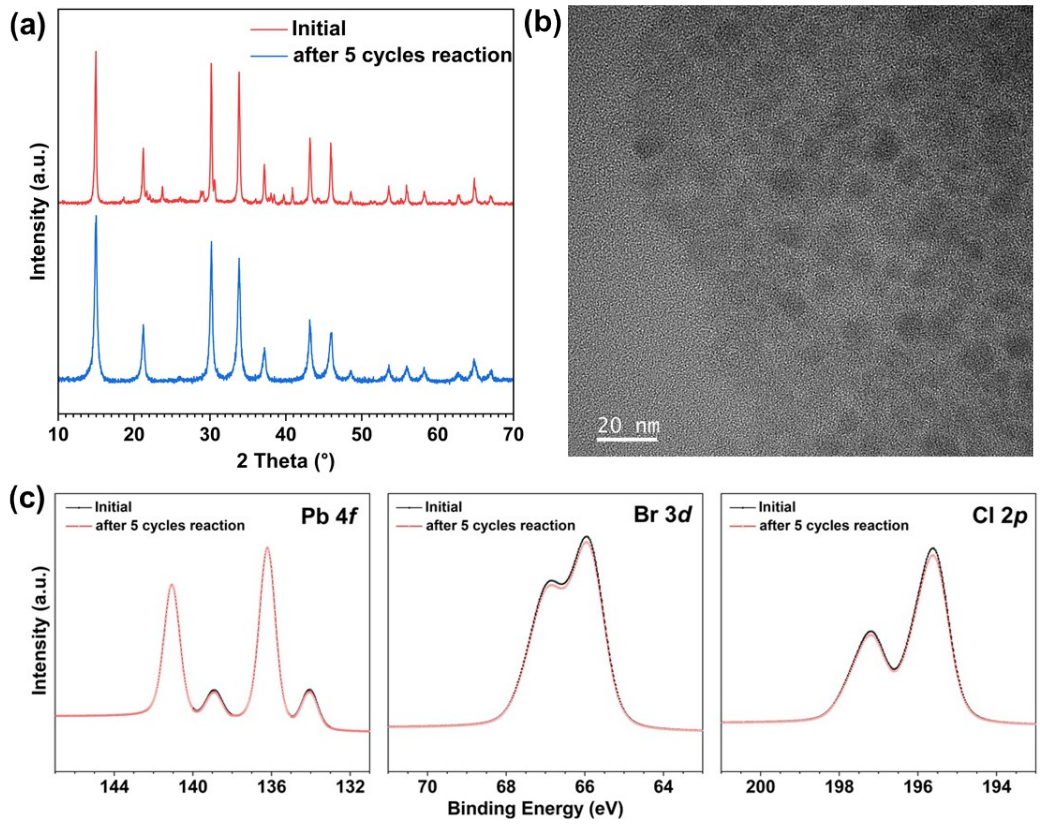

Figure S5. (a) XRD patterns, (b) TEM images and (c) XPS spectra of initial and recycled $MAPbBr_2Cl_1$ QDs as indicated.

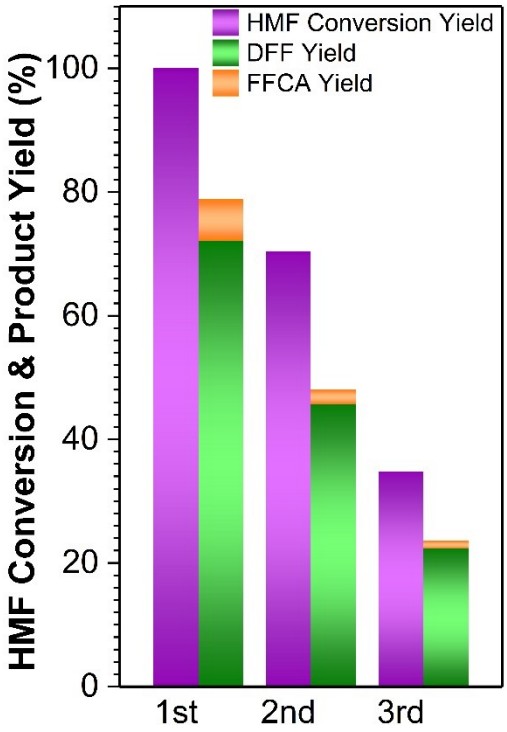

Figure S6. Recycle tests result of $MAPbBr_2Cl_1$ QDs capped with octanoic acid and octylamine. Reaction conditions: 5-hydroxymethylfurfural (HMF) (12.5 μmol), catalyst (4.5 mg), Ethyl acetate (2.5 mL), and 7.1 W blue light-emitting diodes.

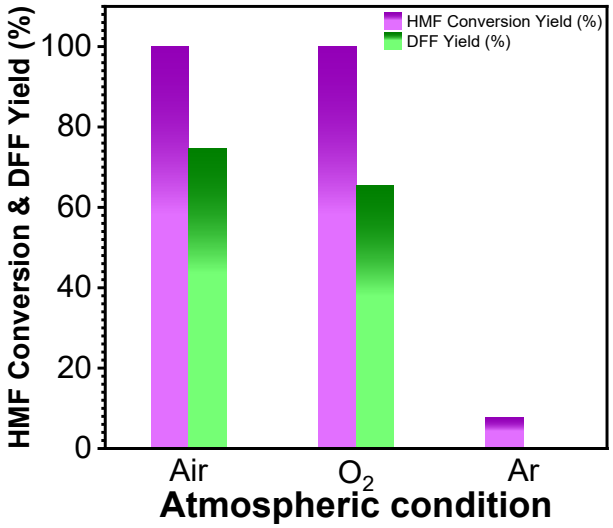

Figure S7. Various atmosphere condition for photocatalytic reaction using $MAPbBr_2Cl_l$ QDs.

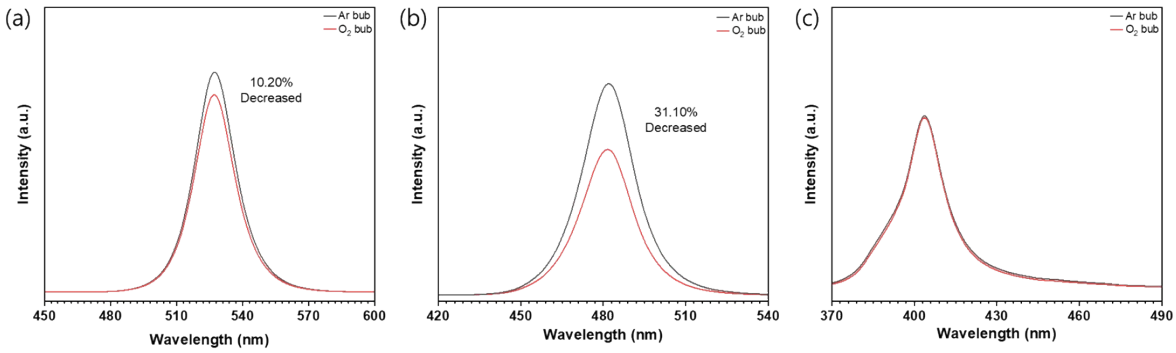

Figure S8. Photoluminescence (PL) quenching of (a) $MAPbBr_3$ QD (a) $MAPbBr_2Cl_1$ QD (b) $MAPbCl_3$ QD with and without O_2.

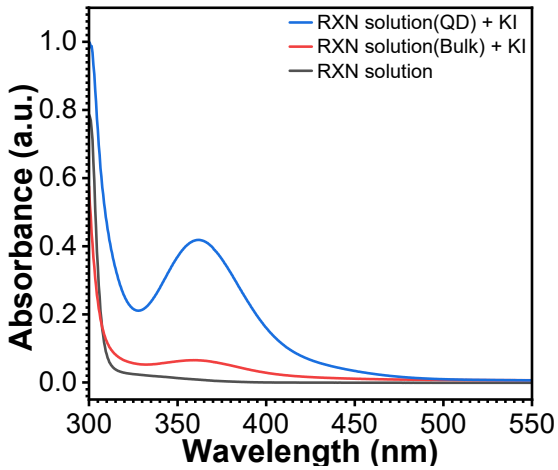

Figure S9. Absorption spectra of in the presence of KI for indicating H_2O_2 generation as photocatalytic reaction progress using $MAPbBr_2Cl_l$ QDs, bulk $MAPbBr_2Cl_l$ and absence of photocatalyst.

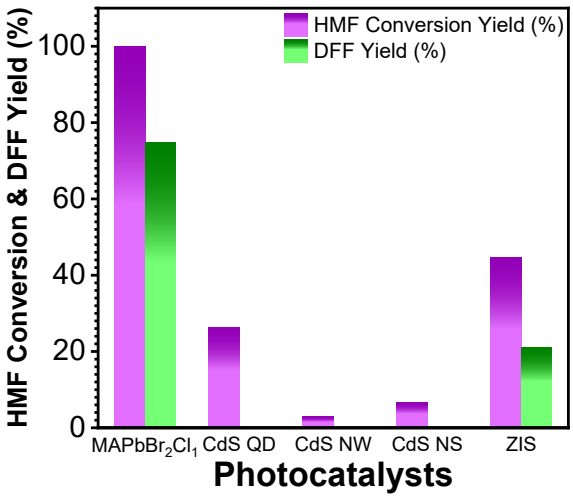

Figure S10. Comparison with CdS QDs, decorated CdS and Zinc Indium sulfide nanoparticles

Table S1. The surface to inner concentration ratio of Br^- and Cl^- ions in the $MAPbBr_xCl_{3-x}$ QDs.

	Br 3d		Cl 2p	
$MAPb(Br_xCl_{1-x})_3$	Inner	Surface	Inner	Surface
-Br_3	1	0.21116	-	-
-$Br_{2.5}Cl_{0.5}$	1	0.21109	1	0.41969
-Br_2Cl_1	1	0.21010	1	0.41977
-$Br_{1.5}Cl_{1.5}$	1	0.20991	1	0.41989
-Br_1Cl_2	1	0.20988	1	0.42001
-Cl_3	-	-	1	0.42118

Table S2. Comparison of photocatalytic efficiency with other literatures.

Catal.	Light Source	Conversed HMF (μmole)	RXN Time (hr)	Catal. (mg)	Efficiency (μmole/mg·h)	Ref.
UCNT	300 W Xe lamp (>420 nm)	50.000	5	100	0.1000	S1
g-C_3N_4	300 W Xe lamp (>360 nm)	85.600	6	50	0.2853	S2
SGCN	Solar simulator (>400 nm, 100 mW/cm^2)	13.800	6	10	0.2300	S3
$Zn_{0.5}Cd_{0.5}S$ @1wt% MnO_2	30 W WLED (>400 nm)	7.391	24	20	0.0154	S4
TBA-W_{10}	Xe lamp (400 mW/cm^2)	4.910	2	2.5	0.9820	S5
MCN-540 (g-C_3N_4)	Natural solar light	37.125	4	25	0.3713	S6
TEO PCN-H_2O_2	Natural solar light	13.875	4	50	0.0694	S7
Nb_2O_5	300 W Xe lamp	0.096	6	50	0.0003	S8
4.7%WO_3/gC_3N_4	300 W Xe lamp	0.242	6	50	0.0008	S9
CTF-Th/SBA15	460 nm Blue LED (65 mW/cm^2)	57.000	30	10	0.1900	S10
SGH-TiO_2	Visible	11.8	4	20	0.1475	S11
MIL-53(Fe) (CM-10)	>360 nm Blue LED	76.5	6	50	0.2550	S12
CN-WO_3@MnO_2	420 nm LED (10 W)	11.64	24	15	0.0323	S13
12% Bi_2WO_6/ mpg-C_3N_4	300 W Xe lamp (>400 nm)	0.297	8	50	0.0007	S14
TMADT	35 W Visible light (W/Bromine)	91.8	12	5.3	1.4434	S15
$ZnIn_2S_4$ 2D	Blue LED (λmax=467 nm)	38	2	10	1.9000	S16
$MAPbBr_2Cl_1$ QD	445 nm Blue LED	12.500	1.5	4.5	1.8519	**This study**

References

S1. X. Bao, M. Liu, Z. Wang, D. Dai, P. Wang, H. Cheng, Y. Liu, Z. Zheng, Y. Dai and B. Huang, *ACS Catal.*, 2022, **12**, 1919-1929.

S2. Q. Wu, Y. He, H. Zhang, Z. Feng, Y. Wu and T. Wu, *Mol. Catal.*, 2017, **436**, 10-18.

S3. V. R. Battula, A. Jaryal and K. Kailasam, *J. Mater. Chem. A*, 2019, **7**, 5643-5649.

S4. S. Dhingra, T. Chhabra, V. Krishnan and C. M. Nagaraja, *ACS Appl. Energy Mater.*, 2020, **3**, 7138-7148.

S5. Z. Li, M. Zhang, X. Xin and H. Lv, *ChemCatChem*, 2021, **13**, 1389-1395.

S6. I. Krivtsov, E. I. García-López, G. Marcì, L. Palmisano, Z. Amghouz, J. R. García, S. Ordóñez and E. Díaz, *Appl. Catal. B: Environ.*, 2017, **204**, 430-439.

S7. M. Ilkaeva, I. Krivtsov, E. I. García-López, G. Marcì, O. Khainakova, J. R. García, L. Palmisano, E. Díaz and S. Ordóñez, *J. Catal.*, 2018, **359**, 212-222.

S8. H. Zhang, Q. Wu, C. Guo, Y. Wu and T. Wu, *ACS Sustain. Chem. Eng.*, 2017, **5**, 3517-3523.

S9. H. Zhang, Z. Feng, Y. Zhu, Y. Wu and T. Wu, *J. Photochem. Photobiol. A*, 2019, **371**, 1-9.

S10. C. Ayed, W. Huang, G. Kizilsavas, K. Landfester and K. A. I. Zhang, *ChemPhotoChem*, 2020, **4**, 571-576.

S11. A. Khan, M. Goepel, A. Kubas, D. Lomot, W. Lisowski, D. Lisovytskiy, A. Nowicka, J. C. Colmenares and R. Glaser, *ChemSusChem*, 2021, **14**, 1351-1362.

S12. D. Huang, H. Wang and Y. Wu, *Molecules*, 2022, **27**, 8537.

S13. H. Qian, Q. Hou, W. Zhang, Y. Nie, R. Lai, H. Ren, G. Yu, X. Bai, H. Wang and M. Ju, *Appl. Catal. B: Environ.*, 2022, **319**, 121907.

S14. L. Cheng, D. Huang, Y. Zhang and Y. Wu, *Appl. Organomet. Chem.*, 2021, **35**, e6404.

S15. B. Yang, W. Hu, F. Wan, C. Zhang, Z. Fu, A. Su, M. Chen and Y. Liu, *Chem. Eng. J.*, 2020, **396**, 125345.

S16. S. Ding, J. B. Gabriel Filho, T. Peppel, S. Haida, J. Rabeah, N. Steinfeldt and J. Strunk, *Sustain. Energy Fuels*, 2023, **7**, 4396-4400.