

Supporting information

Earth-abundant and Environment Friendly Organic-inorganic Hybrid Tetrachloroferrate Salt $\text{CH}_3\text{NH}_3\text{FeCl}_4$: Structure, Adsorption Properties and Photoelectric Behavior

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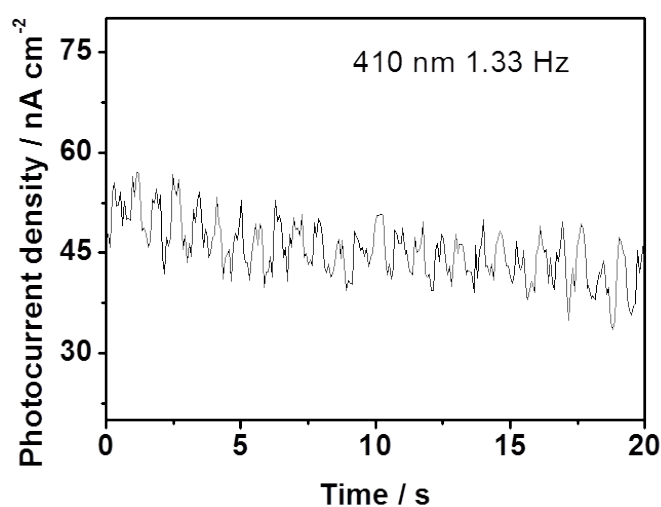


Figure S1 photocurrent density-time characteristics of the FTO/TiO₂/MAFeCl₄/carbon electrode device under 410 nm with flashlight frequency 1.33 Hz.

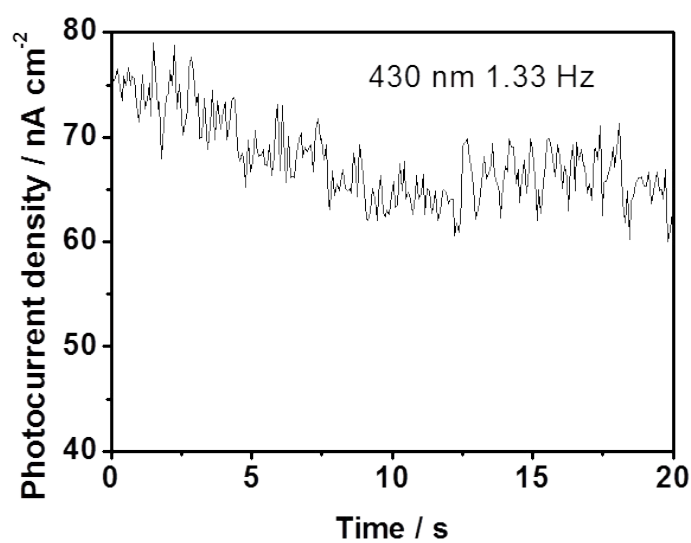


Figure S2 photocurrent density-time characteristics of the FTO/TiO₂/MAFeCl₄/carbon electrode device under 430 nm with flashlight frequency 1.33 Hz.

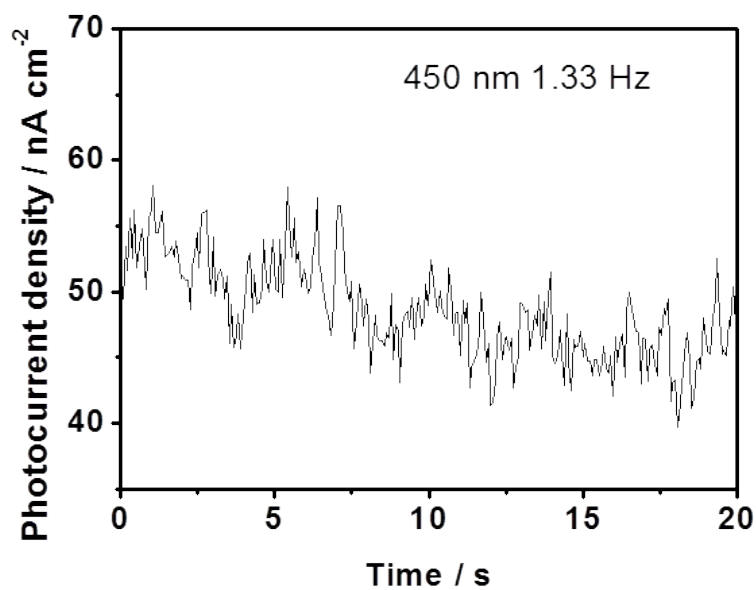


Figure S3 photocurrent density-time characteristics of the FTO/TiO₂/MAFeCl₄/carbon electrode device under 450 nm with flashlight frequency 1.33 Hz.

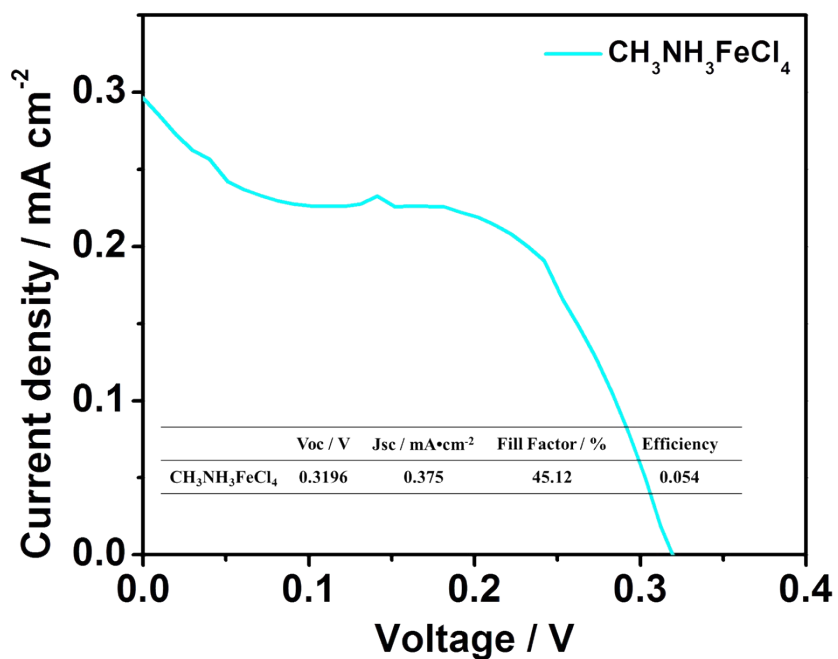


Figure S4 The best photocurrent density-voltage curve of the FTO/TiO₂/MAFeCl₄/carbon electrode device under AM 1.5 (100 mW / cm²)

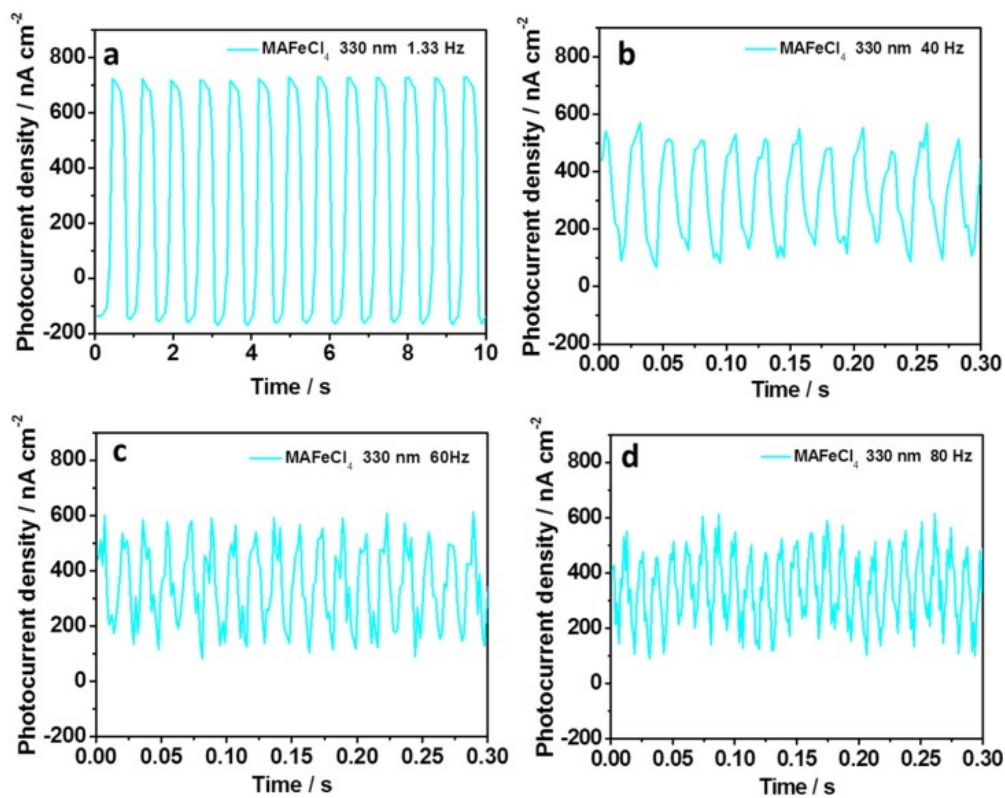


Figure S5 Photocurrent density-time characteristics of the FTO/TiO₂/MAFeCl₄/carbon electrode device under different flashlight frequencies (1.33, 40, 60 and 80 Hz) with 330 nm light-beam.

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for CH₃NH₃FeCl₄. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	895(1)	7500	8027(1)	58(1)
Cl(1)	882(1)	5072(2)	6772(1)	87(1)
Cl(2)	2512(2)	7500	9166(2)	96(1)
Cl(3)	-606(2)	7500	9324(2)	131(1)
N(1)	1509(6)	7500	2299(6)	129(3)
C(1)	1757(7)	7500	3653(8)	93(2)

Table S2. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for CH₃NH₃FeCl₄. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U12	U13	U23
Fe(1)	66(1)	52(1)	56(1)	0	-1(1)	0
Cl(1)	105(1)	64(1)	91(1)	-21(1)	-7(1)	-6(1)
Cl(2)	97(1)	105(2)	85(1)	0	-33(1)	0
Cl(3)	110(2)	165(2)	119(2)	0	54(1)	0
N(1)	87(5)	210(10)	90(5)	0	21(4)	0
C(1)	94(6)	101(6)	84(5)	0	-15(4)	0

Table S3 photocurrent density-voltage parameter of the FTO/TiO₂/MAFeCl₄/carbon electrode device under AM 1.5 (100 mW / cm²)

V _{oc} / V	J _{sc} / mA·cm ⁻²	Fill Factor / %	Efficiency
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Mean	0.30949	0.30267	36.45619	0.03286
Standard Deviation	0.02072	0.06708	9.41458	0.00784
