Supporting information

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

Jie Yin, a,∗ Shaozhen Shi, a Jiazhen Wei, a Guohang He, a Lin Fan, a Junxue Guo, a Kaixuan Zhang, a Wenli Xu, a Cang Yuan, a Yunying Wang, a Liwen Wang, a Xipeng Pu, a Wenzhi Li, a Dafeng Zhang, a Jie Wang, a Xiaozhen Ren, a Huiyan Ma, a Xin Shao, a Huawei Zhou a,∗

aCollege of Materials Science and Engineering, Liaocheng University; School of Chemistry and Chemical Engineering, Liaocheng University; Shandong Provincial Key Laboratory of Chemical Energy Storage and Novel Cell Technology, Liaocheng 252059, China.

Figure S1 photocurrent density-time characteristics of the FTO/TiO$_2$/MAFeCl$_4$/carbon electrode device under 410 nm with flashlight frequency 1.33 Hz.
Figure S2  photocurrent density-time characteristics of the FTO/TiO$_2$/MAFeCl$_4$/carbon electrode device under 430 nm with flashlight frequency 1.33 Hz.

Figure S3  photocurrent density-time characteristics of the FTO/TiO$_2$/MAFeCl$_4$/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)
Photocurrent density-time characteristics of the FTO/TiO$_2$/MAFeCl$_4$/carbon electrode device under different flashlight frequencies (1.33, 40, 60 and 80 Hz) with 330 nm light-beam.

Table S1. Atomic coordinates (× 10$^4$) and equivalent isotropic displacement parameters (Å$^2$ × 10$^3$) for CH$_3$NH$_3$FeCl$_4$. U(eq) is defined as one third of the trace of the orthogonalized Uij 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 (Å$^2$ × 10$^3$) for CH$_3$NH$_3$FeCl$_4$. The anisotropic displacement factor exponent takes the form: -2π$^2$ [ h$^2$ a$^*$ U$_{11}$ + ... + 2 h k a$^*$ b$^*$ U$_{12}$ ]

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

Table S3 photocurrent density-voltage parameter of the FTO/TiO$_2$/MAFeCl$_4$/carbon electrode device under AM 1.5 (100 mW/cm$^2$)

|      | $V_{oc}$/ V | $J_{sc}$/ mA·cm$^{-2}$ | Fill Factor / % | Efficiency |
|------|-------------|------------------------|-----------------|------------|------------|


|                     | Value     | Value     | Value     | Value     |
|---------------------|-----------|-----------|-----------|-----------|
| Mean                | 0.30949   | 0.30267   | 36.45619  | 0.03286   |
| Standard Deviation  | 0.02072   | 0.06708   | 9.41458   | 0.00784   |