Supporting Information

Synthesis, post-synthetic modification and stability of styrylammonium lead iodide hybrid perovskite

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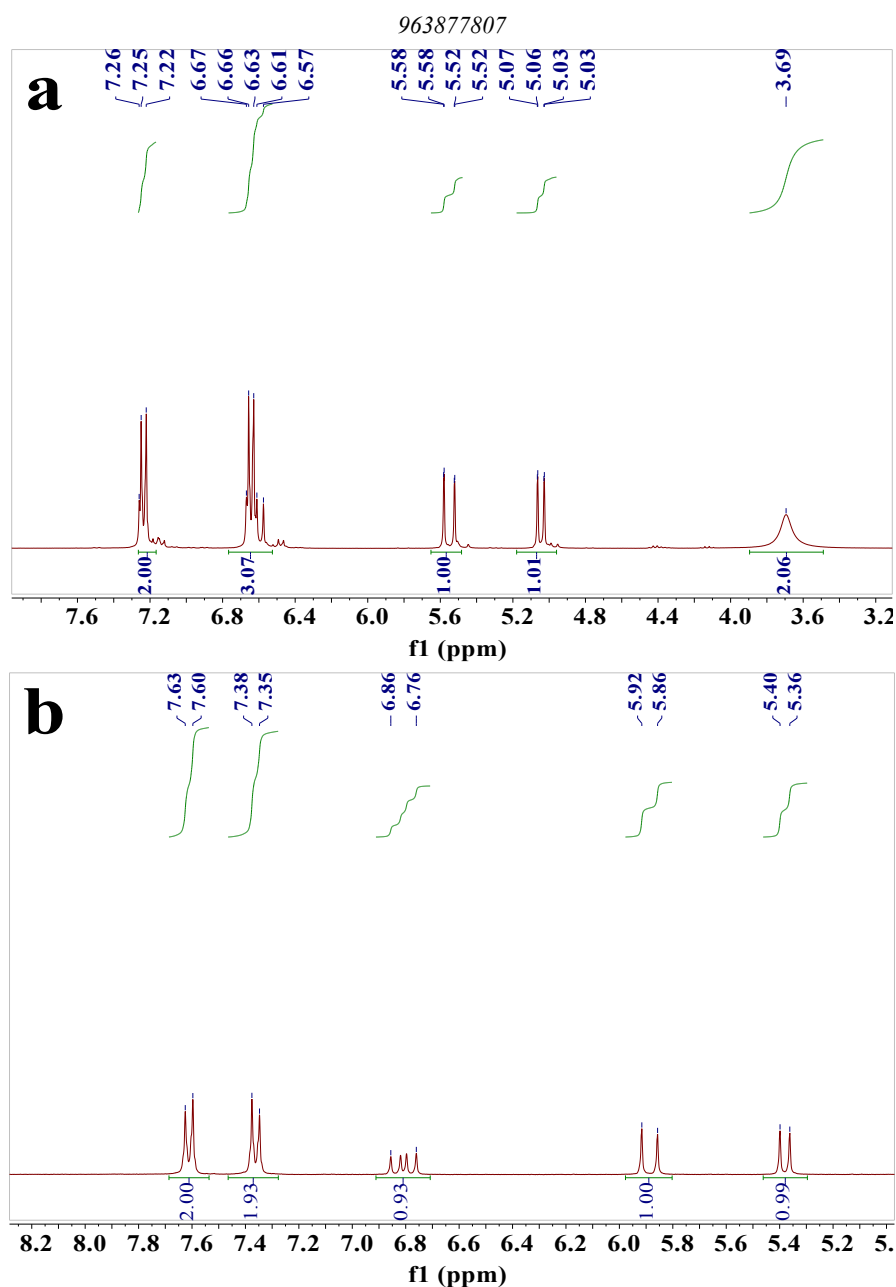
Figure S1. ^{1}H NMR spectra of 4-aminostyrene (a) and styryl ammonium 1 (b) solute in CDCl$_3$ and

D$_2$O, respectively. 4-Aminostyrene ^{1}H NMR: (300MHz, CDCl3), δ=7.25-7.22 (d, 2H; J^3= 8.38,Ar), 6.66-6.63 (d, 2H; J^3=8.37, Ar), 6.67-6.57 (m, H; J^3=10.894 & J^3=17.313, CH=CR), δ=5.58-5.52 (d, H; J^3=17.590, CR=CH$_2$), δ=5.07-5.03(d, H; J^3=10.873, CR=CH$_2$). Styryl ammonium ^{1}H NMR: (300 MHz, D$_2$O) δ=7.50-7.53 (d, 2H; J^3=8.52, Ar), 7.35-7.38 (d, 2H; J^3=8.56, Ar), 6.75-6.86 (m, H; J^3= 17.71 & J^3=10.96, CH=CR), δ=5.86-5.92 (d, H; J^3= 17.71, CR=CH$_2$), δ=5.36-5.40 (d, H; J^3=10.97, CR=CH$_2$).
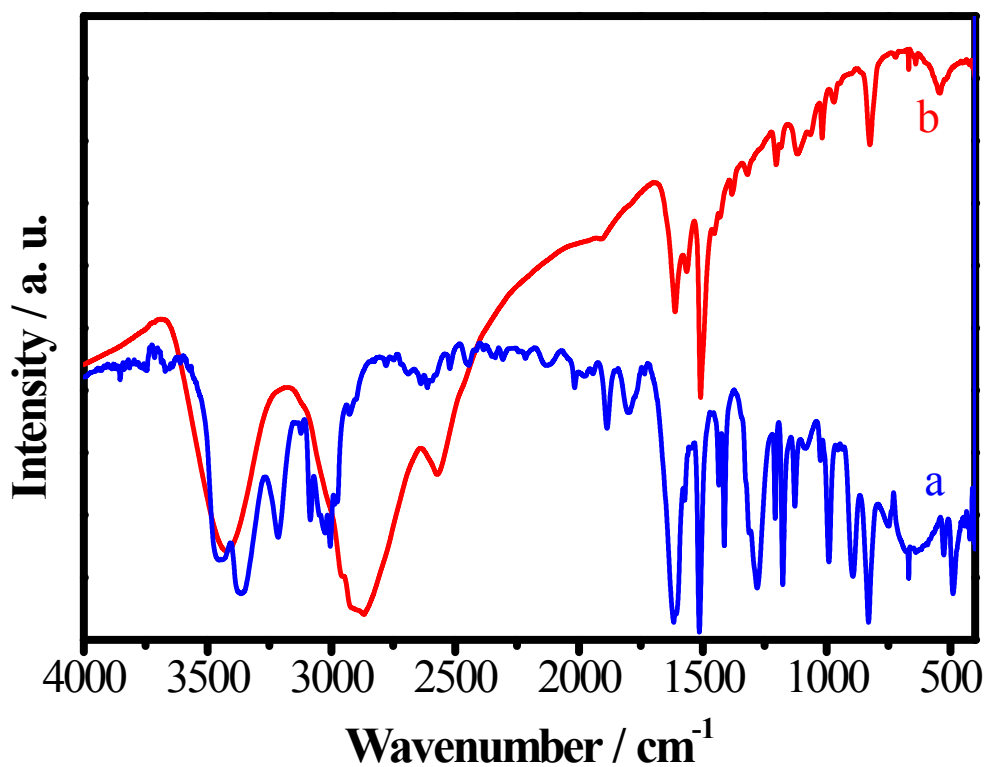

Figure S2. Infrared spectra of 4-aminosyrene (a) and 4-styryl ammonium **1** (b)

Table S1 Chemical composition and empirical formula of HP1 determined by combining X-ray

fluorescence (Pb and I) and combustion elemental analysis (N, C and H).

Item	Pb% (XRF)	N % (EA)	C % (EA)	H % (EA)	I(XRF) %	Rest %
Proportion	34.758	1.16	8.47	1.04	54.189	0.383%
Number of Atoms	1	0.493	4.2	6.19	2.5	-
Formula	$PbI_{2.5}(Amino\text{-}styrene)_{0.5}$					

The fitting parameters of CPS analysis are: applied voltage 20 kV, working distance 6 mm,
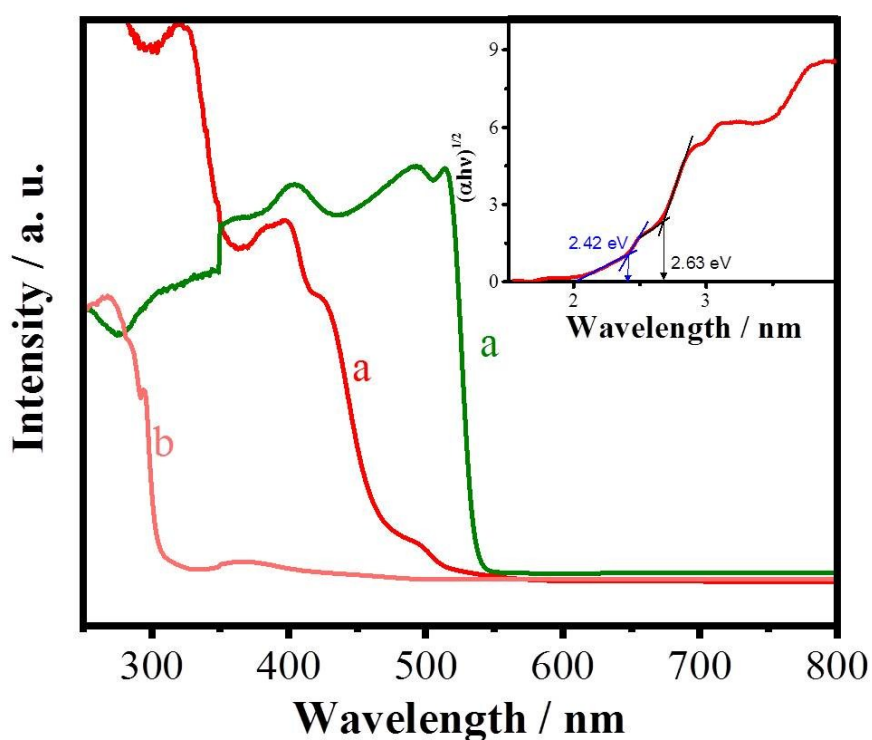
aperture 30 μm, input count rate 6410 and death time 18%.

Figure S3. UV-Vis diffuse reflectance spectra of commercial PbI_2 (a), 4-styryl ammonium powder
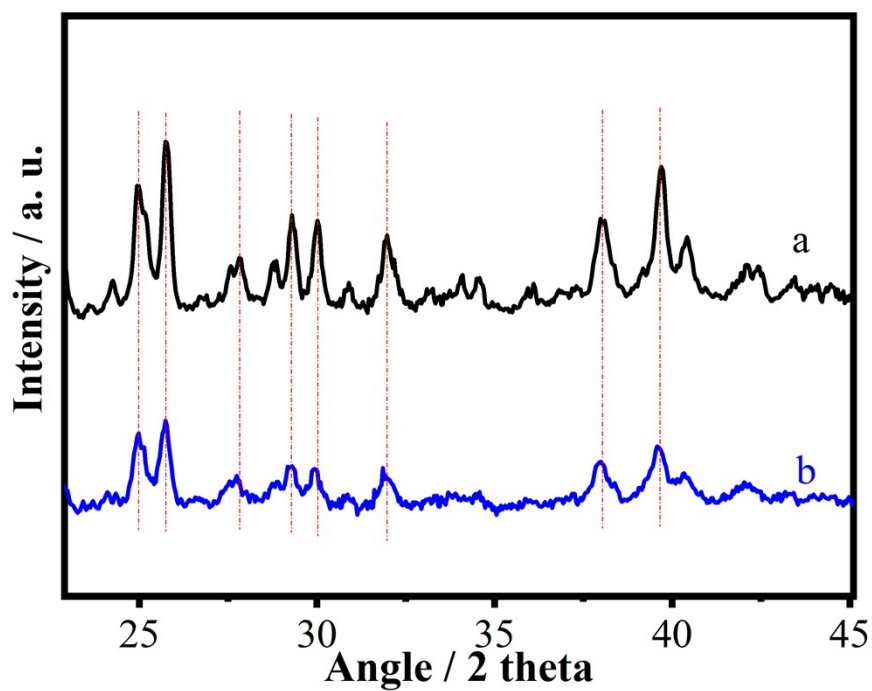(b) and HP1 material (c). Inset shows the Tauc plot of HP1.

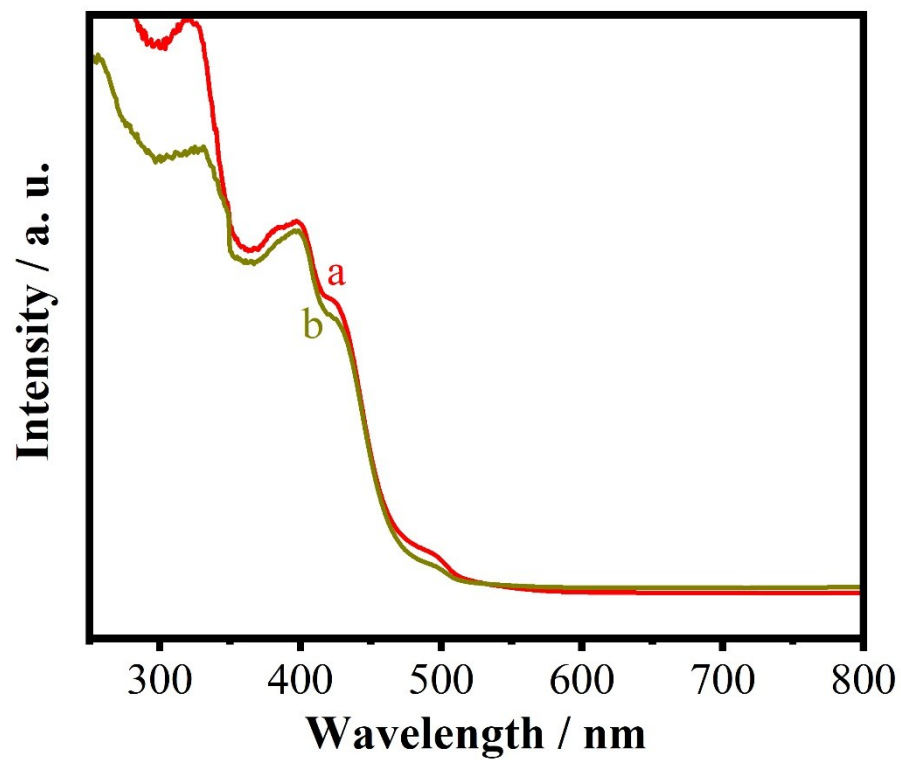**Figure S4.** X-ray diffraction patterns of HP1 (a) and HP2 (b).

Figure S5. UV-vis diffuse reflectance spectroscopy of HP1 (a) and HP2 (b).
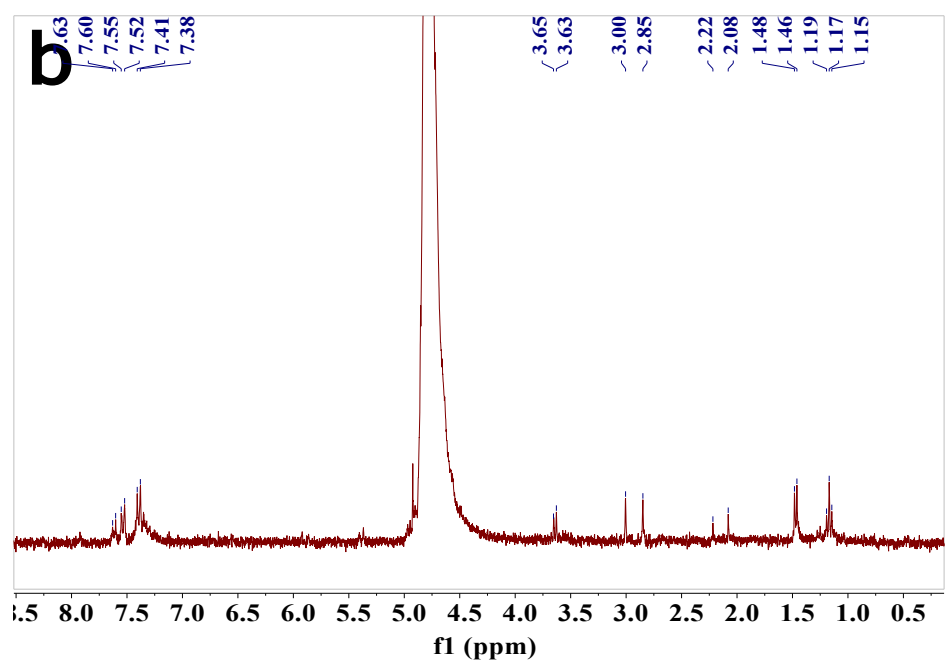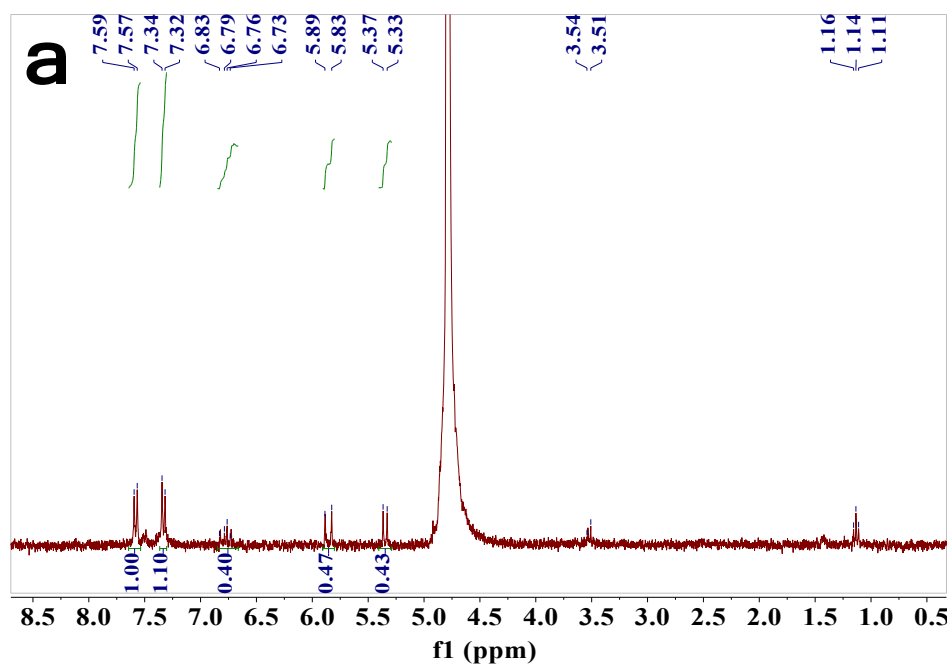
Figure S6. ^{1}H NMR spectra of organic ammonium samples extracted from HP1 (a) and HP2 (b) using D_2O.
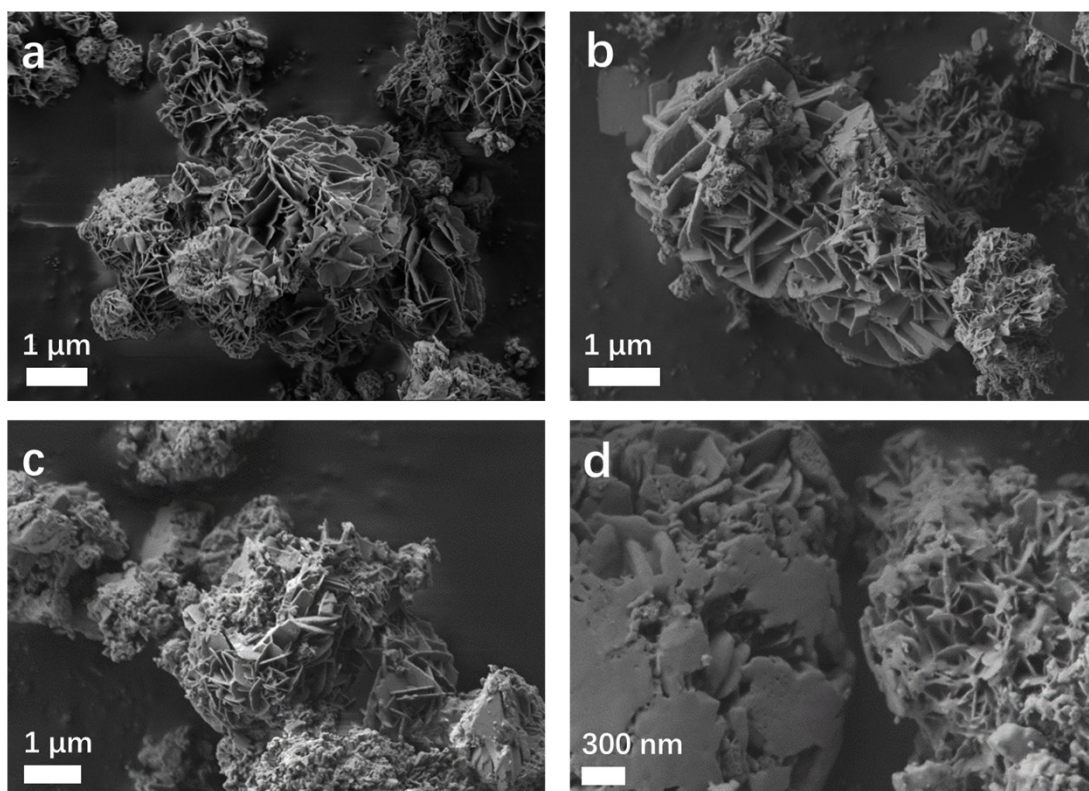
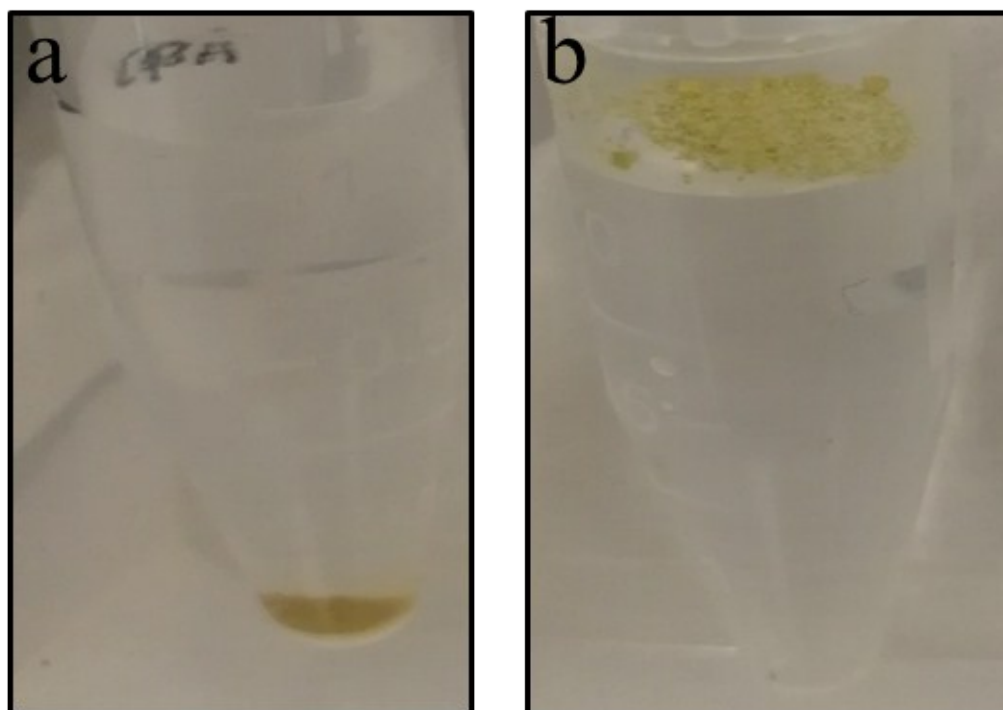Figure S7 Representative SEM images of HP1 (a), (b) and HP2 (c), (d).

Figure S8. H_2O hydrophobicity test of HP1 (a) and HP2 (b). It can be seen that HP1 precipitates
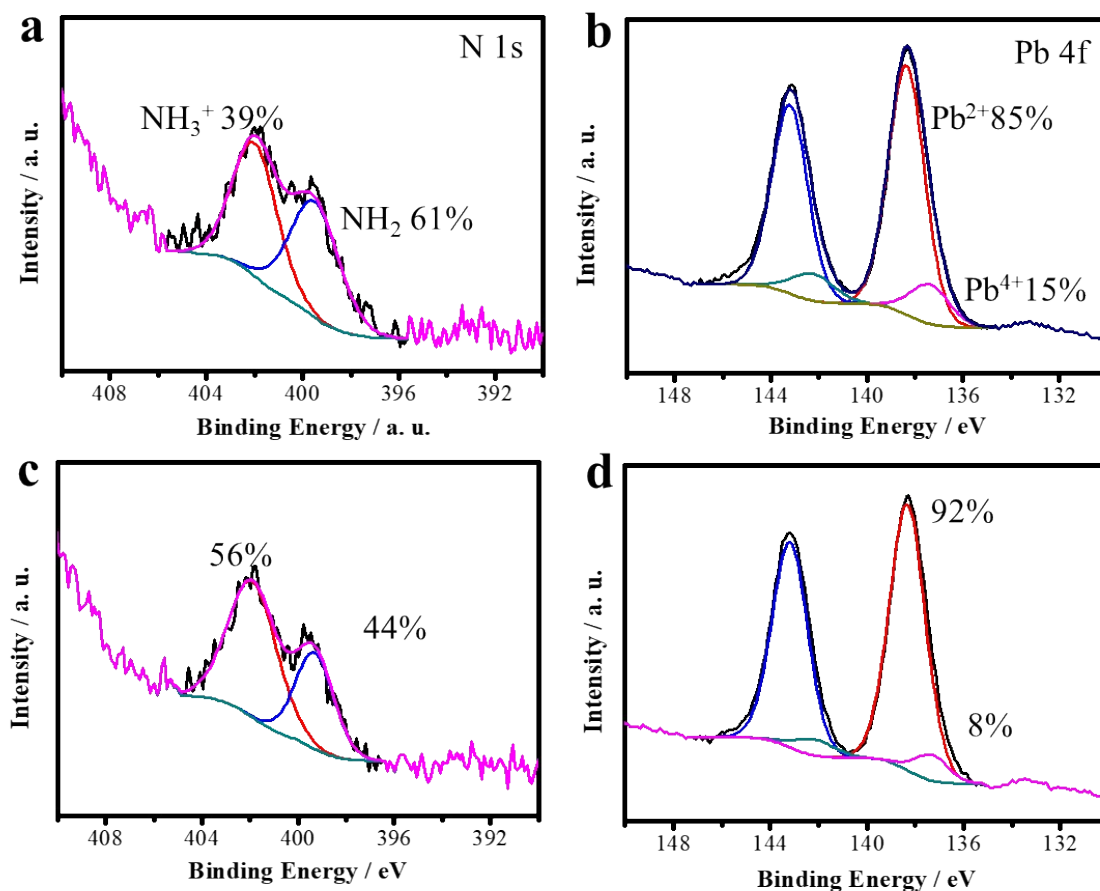
on the bottom, while HP2 floats on water.

Figure S9. XPS N1s and Pb4f spectra obtained from HP1 samples: after illumination ($\lambda > 400$ nm) with O_2 (a and b) or in the absence of O_2 (c and d) for 20 h.

Calculation of valence band edge

All the XPS spectra were obtained with Al as the X-ray source. The valence band spectrum was first calibrated by C1s (284.8 eV), The valence band edge position was determined by intersection of tangent line and baseline of the valence band lowest energy peak, giving a value of 1.11 eV. The obtained value refers to the valence band energy versus to Fermi level, E_B^F.

The valence band edge to vacuum E_B^V can be calculated according to the following formula:

$$E_B^V = E_B^F + \phi_{sp}$$

in which ϕ_{sp} is the work function of the XPS apparatus (4.244 eV). So, the valence band position (versus vacuum) can be obtained as follow:

$$E_B^V = -(1.11 + 4.244)eV = -5.344\ eV$$