Supporting Information

Theoretical Prediction and Experimental Synthesis of $Ba_{0.5}Pb_{0.5}S$ Alloy by Molecular Precursor Route

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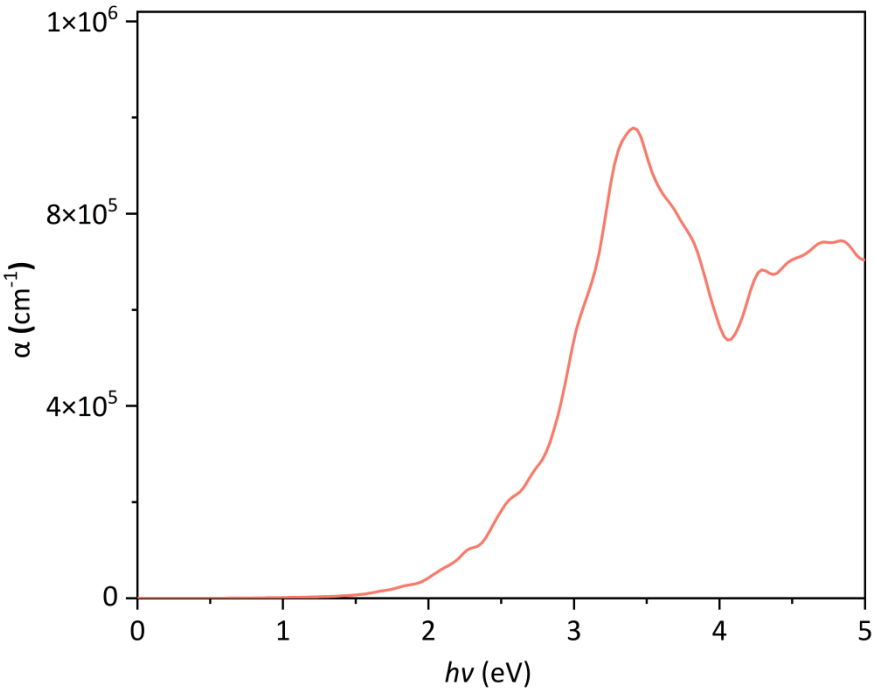

Figure S1. Theoretical absorption spectra for $Ba_{0.5}Pb_{0.5}S$ in X, Y and Z directions.

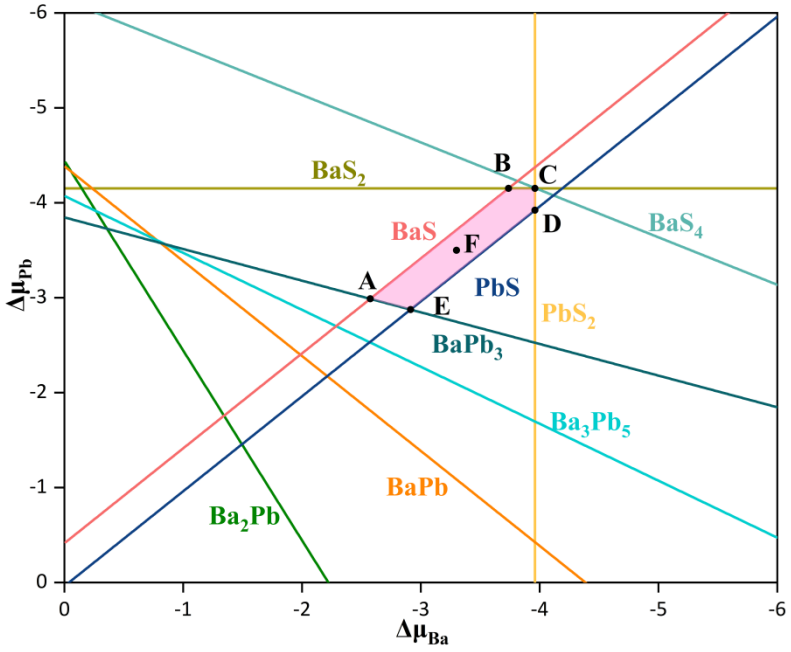

Figure S2. Stable chemical potential region of $Ba_{0.5}Pb_{0.5}S$.

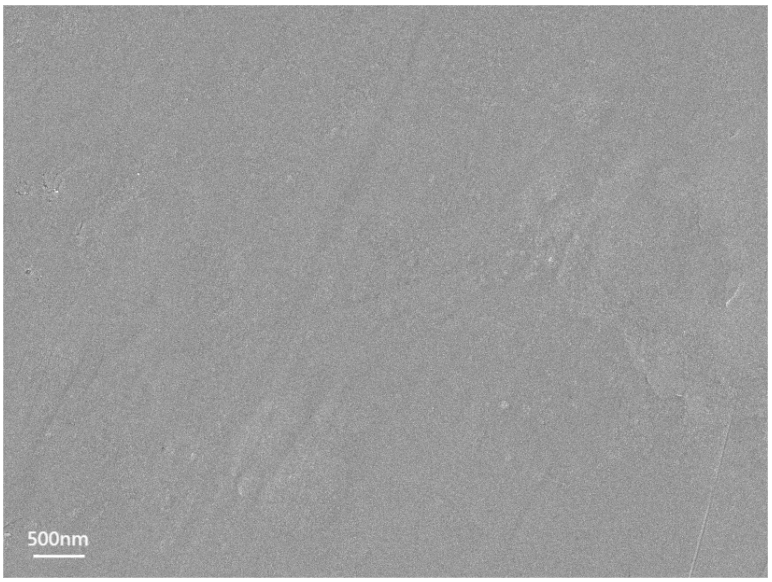

Figure S3. SEM image of $Ba_{0.5}Pb_{0.5}S$ thin film.

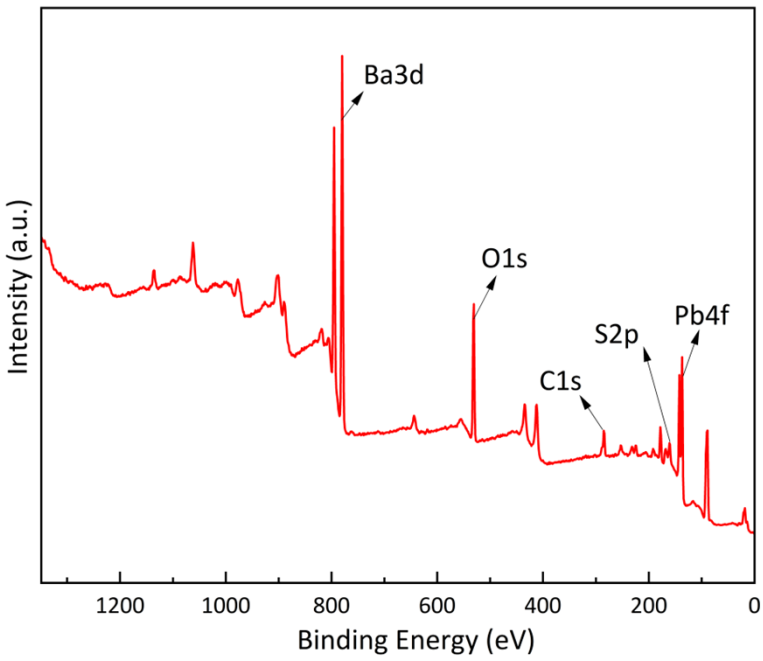

Figure S4. XPS spectra of $Ba_{0.5}Pb_{0.5}S$.

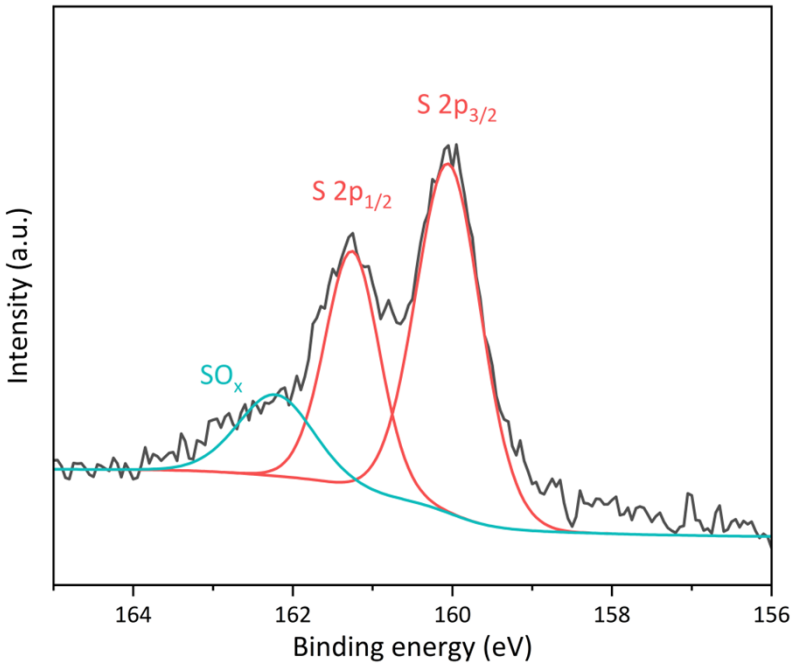

Figure S5. XPS spectra of S 2p.

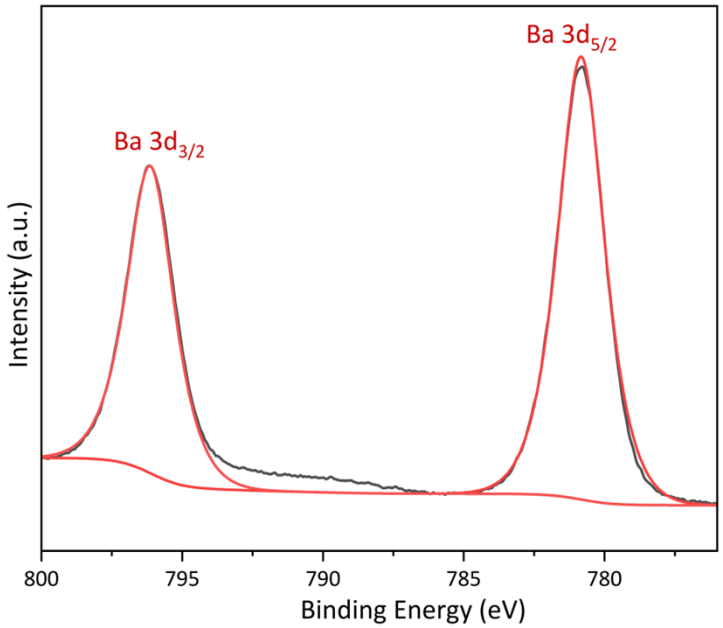

Figure S6. XPS spectra of Ba 3d.

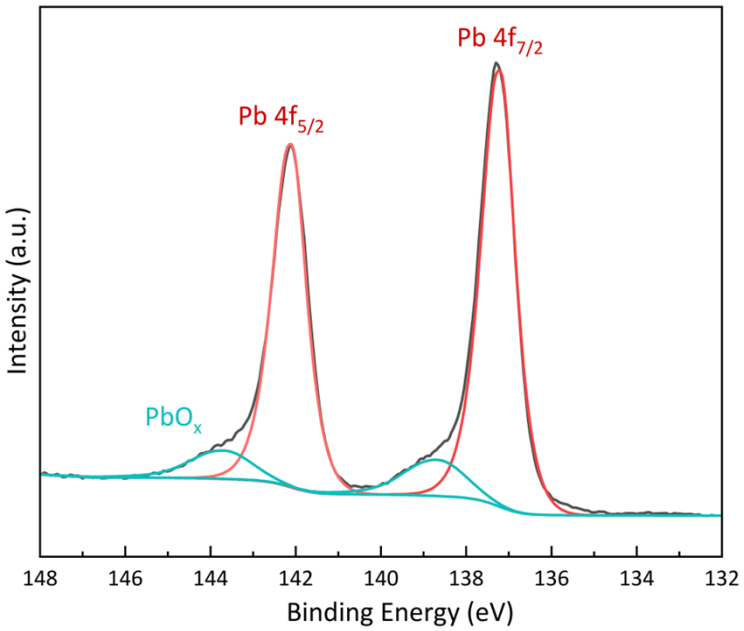

Figure S7. Pb 4f XPS spectra.

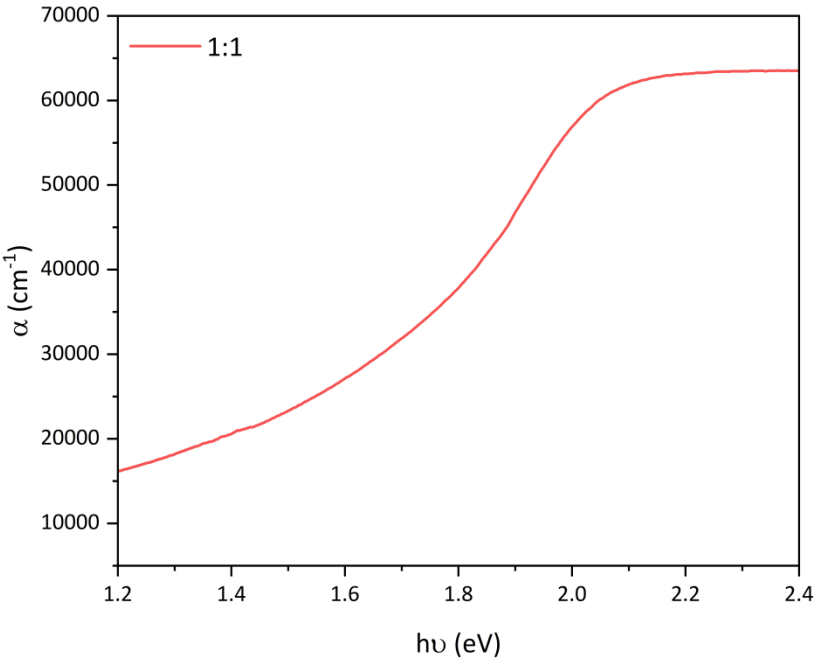

Figure S8. Plot of absorption coefficient (α) as a function of hυ.

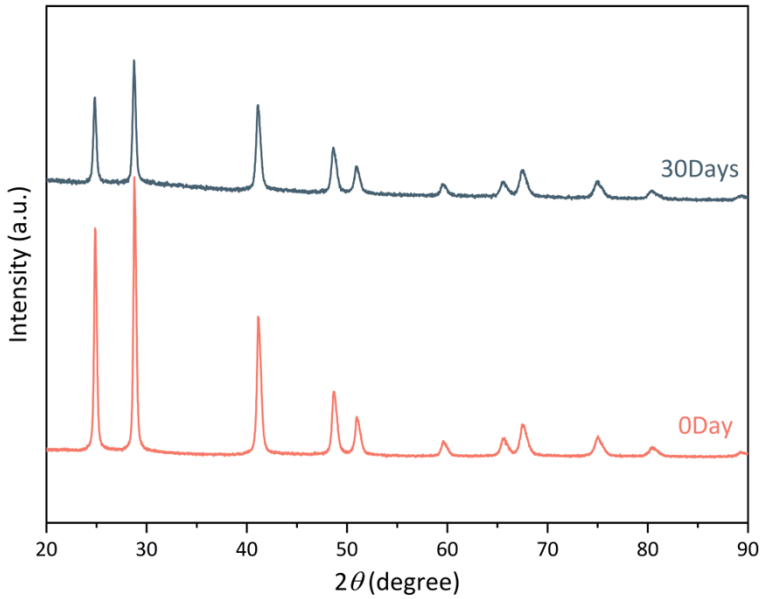

Figure S9. $Ba_{0.5}Pb_{0.5}S$ storage stability test under high-humidity condition.

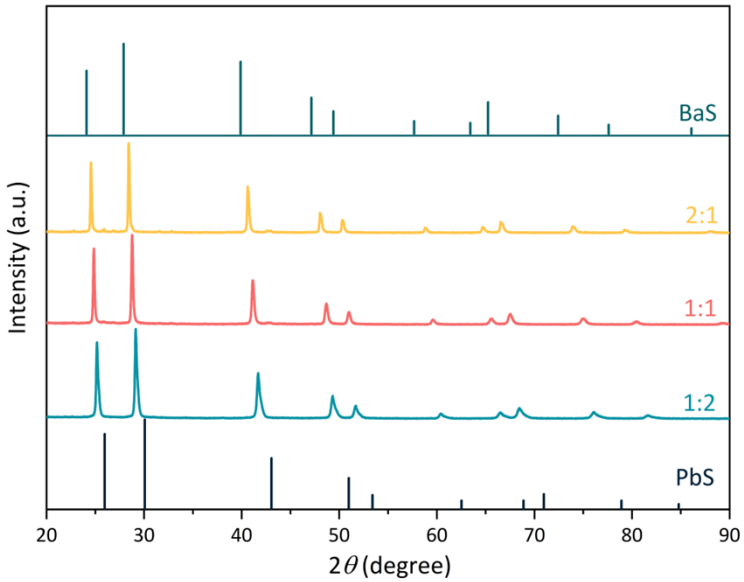

Figure S10. XRD of Ba-Pb-S alloys with different Ba-Pb feed ratios.

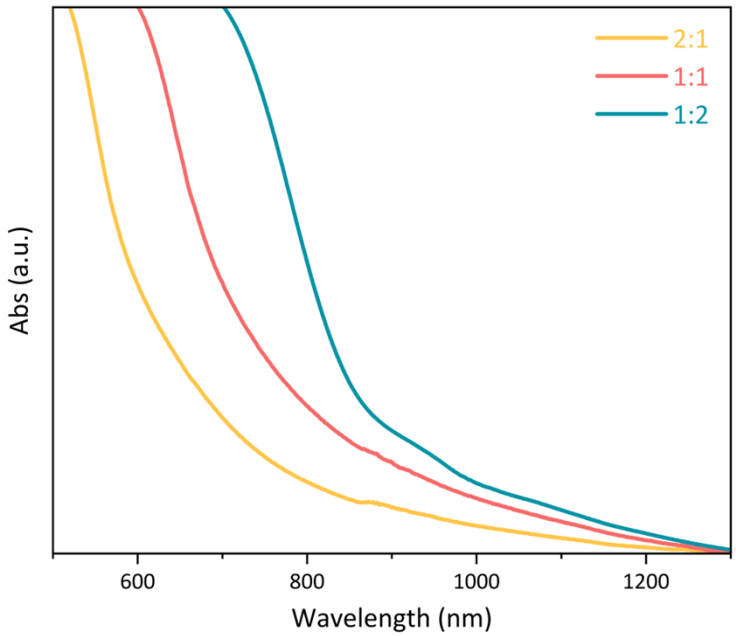

Figure S11. Absorption spectrum of Ba-Pb-S alloys with different Ba-Pb feed ratios.

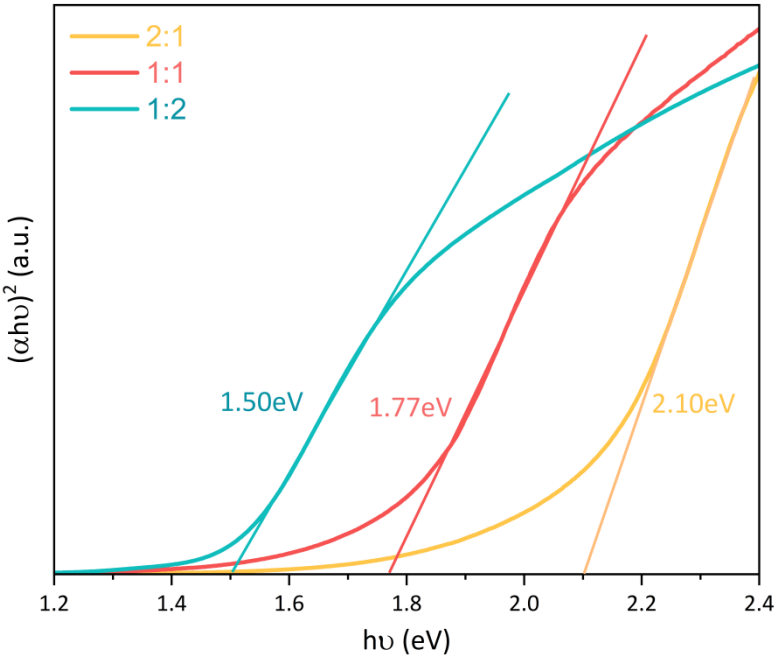

Figure S12. Band gap estimation of Ba-Pb-S alloys with different Ba-Pb feed ratios.

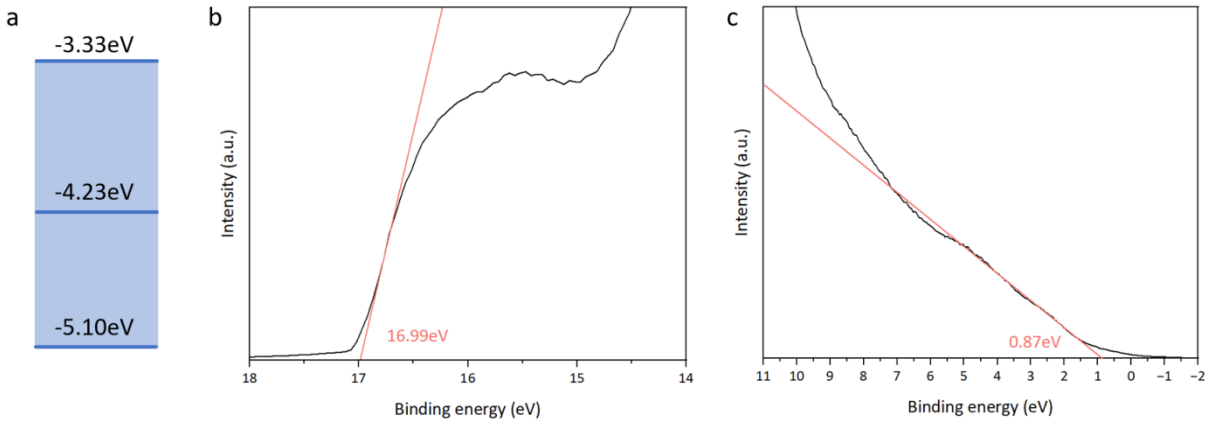

Figure S13. Energy level diagram (a) and UPS spectrum (b,c) of $Ba_{0.5}Pb_{0.5}S$.

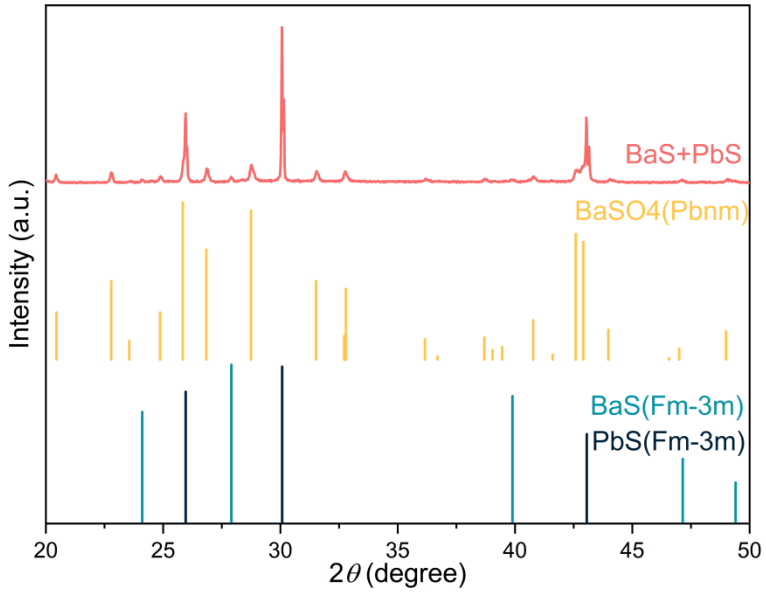

Figure S14. XRD of the powder obtained by grinding BaS powder and PbS powder homogeneously and then reacting at 700°C for 4 hrs.

Table S1. ICP data of $Ba_{0.5}Pb_{0.5}S$.

	Ba 138 ($\times10^{-3}$mg/L)	Pb 208 ($\times10^{-3}$mg/L)
Standard 1	5.000	5.000
Standard 2	9.967	10.022
Standard 3	49.970	50.019
Standard 4	100.013	99.467
Blank	0.209	0.062
Sample	210.383	290.460

Table S2. Comparison of crystal spacing and cell parameter data for BaS, PbS, and $Ba_{0.5}Pb_{0.5}S$ from XRD, along with crystal spacing data for $Ba_{0.5}Pb_{0.5}S$ from HAADF-STEM.

Materials	(h k l)				Cell parameters a=b=c
	200		220		
	2θ(°)	d(nm)	2θ(°)	d(nm)	
BaS	27.91	0.319	39.89	0.226	6.386
PbS	30.07	0.297	43.06	0.210	5.936
$Ba_{0.5}Pb_{0.5}S$	28.83	0.309#	41.14	0.219#	6.180

#Data obtained from HAADF-STEM.

Table S3. XPS data of $Ba_{0.5}Pb_{0.5}S$.

Element	Peak Splitting (eV)	Peak ID	Binding energy (eV)
Ba	15.4	$3d_{5/2}$	780.8
		$3d_{3/2}$	796.2
Pb	4.9	$4f_{7/2}$	137.2
		$4f_{5/2}$	142.1
PbO_x	4.9	$4f_{7/2}$	138.8
		$4f_{5/2}$	143.7
S	1.2	$2p_{3/2}$	160.1
		$2p_{1/2}$	161.3
SO_x		2p	162.3