Electronic Supplementary information (ESI)

PbI_2 Band Gap Engineering by Gel Incorporation

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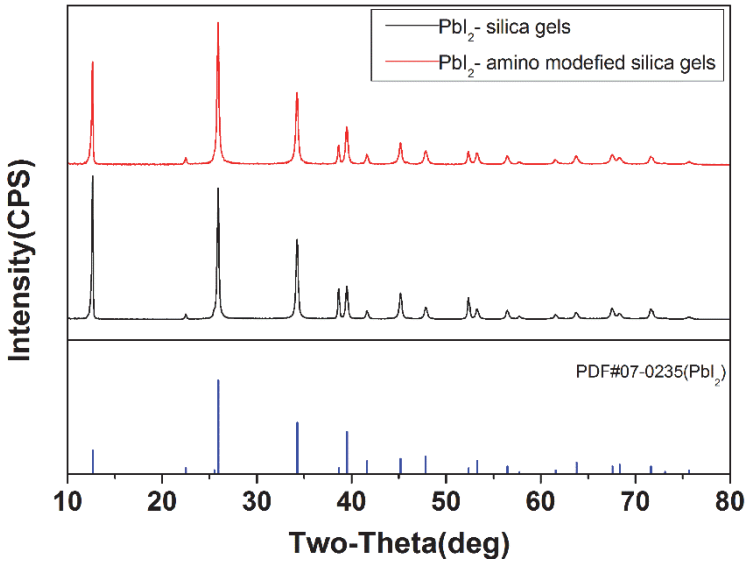

Figure S1. PXRD patterns of PbI_2 grown from 5 w/v% gel and 10 v/v% gel (5% NH_2).

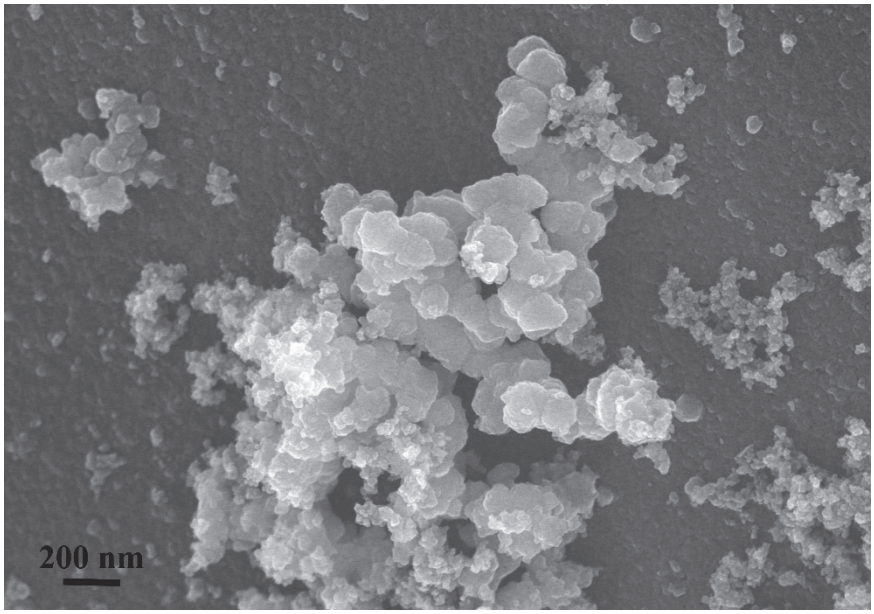

Figure S2. SEM image of exposed colloidal silica particles after etching PbI_2 single crystal grown from 5 w/v% gel.

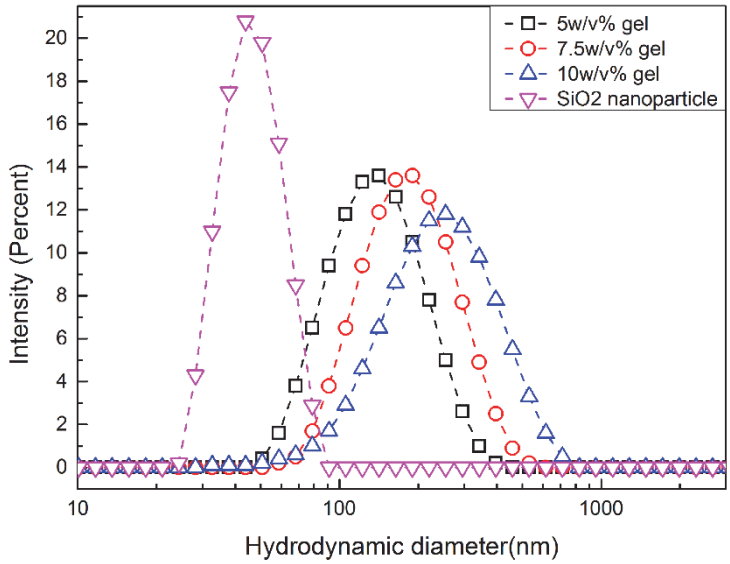

Figure S3. Size distribution of the purchased silica nanoparticles and the colloidal silica particles diluted from the prepared silica gels with varied gel concentrations by intensity examined by DLS.

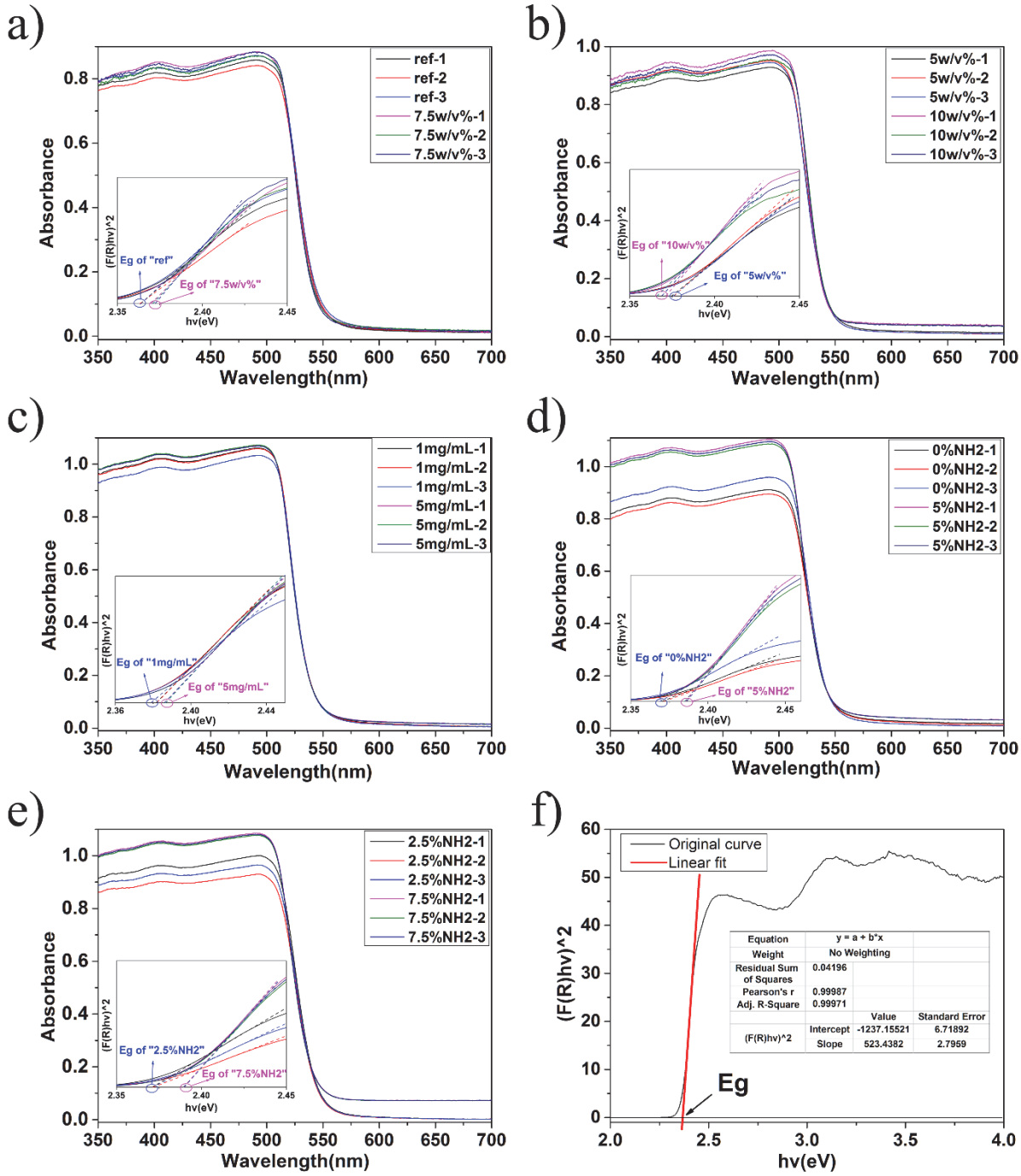

Figure S4. (a-e) Diffuse reflectance spectra of all the samples used in this work drawing with the original measured data. Three samples were prepared and measured for each crystallization condition. Absorbance (A) can be converted to R_∞ by equation $A=-\lg(R_\infty)$. By combining Tauc equation with KM model, the $[F(R_\infty)\ h\nu]^2$ was plotted against the $h\nu$ in (f), taking the spectra of ref-1 as an example. Inset table in (f): linear fitting report. In order to reduce the mapping error, the linear fitting was performed in the linear region with Pearson's r $\geq$0.999. Insets in (a-e): ($[F(R_\infty)\ h\nu]^2$ – $h\nu$) curves and corresponding fitting lines of all the samples. E_g values deduced from these curves are listed in table S3.

Table S1. Preparation of 10 v/v% gel from alkoxides with C_{NH2} of 2.5%, 5% and 7.5%. The density values used for calculation: TMOS (1.023 g/ml), APTMS (1.027 g/mL), PbI_2 (6.16 g/cm^3).

C_{NH2}	Solution A				Solution B	
	TMOS /mL	APTMS /mL	Ethanol /mL	$C_4H_6O_4Pb \cdot 3H_2O$/g	Ethanol /mL	DI water /mL
2.5%	8.84	1.16	80	1.9	8	2
5%	7.74	2.26	80	1.9	8	2
7.5%	6.63	3.37	80	1.9	8	2

Table S2. Lattice parameters of referenced PbI_2 and PbI_2 crystals grown from silica gels with varied gel concentrations deduced by the Rietveld refinement method and lattice strains calculated compared to the referenced PbI_2.

Sample	a(Å)	c(Å)	a-axis strain(%)	c-axis strain(%)
PbI_2 (reference)	4.557(2)	6.981(2)	0.000%	0.000%
PbI_2 (5w/v% gel)	4.560(1)	6.984(1)	0.066%	0.043%
PbI_2 (7.5w/v% gel)	4.558(1)	6.983(1)	0.022%	0.029%
PbI_2 (10w/v% gel)	4.557(1)	6.980(1)	0.000%	-0.014%

Table S3. E_g values of each sample measured by DRS. Three samples were prepared and measured for each crystallization condition. The measured E_g values show good reproducibility with small standard deviation.

Samples	Measured E_g values(eV)			Average E_g value(eV)	Standard Deviation(eV)
	1st	2nd	3rd		
ref	2.364	2.363	2.364	2.364	0.00058
5w/v%	2.375	2.373	2.376	2.375	0.00153
7.5w/v%	2.370	2.371	2.374	2.372	0.00208
10w/v%	2.366	2.368	2.372	2.369	0.00306
1mg/mL	2.382	2.382	2.379	2.381	0.00173
5mg/mL	2.386	2.387	2.386	2.386	0.00058
0%NH_2	2.368	2.37	2.371	2.370	0.00153
2.5%NH_2	2.372	2.372	2.373	2.372	0.00058
5%NH_2	2.384	2.385	2.386	2.385	0.00100
7.5%NH_2	2.389	2.389	2.39	2.389	0.00058