

Supporting Information

Temperature-dependent excited-state for detecting reversible phase transitions in 2D lead(II) iodide perovskites

Mahboubeh Jamshidi, James M. Gardner**

Department of Chemistry, Division of Applied Physical Chemistry, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden.

mahjam@kth.se and jgardner@kth.se

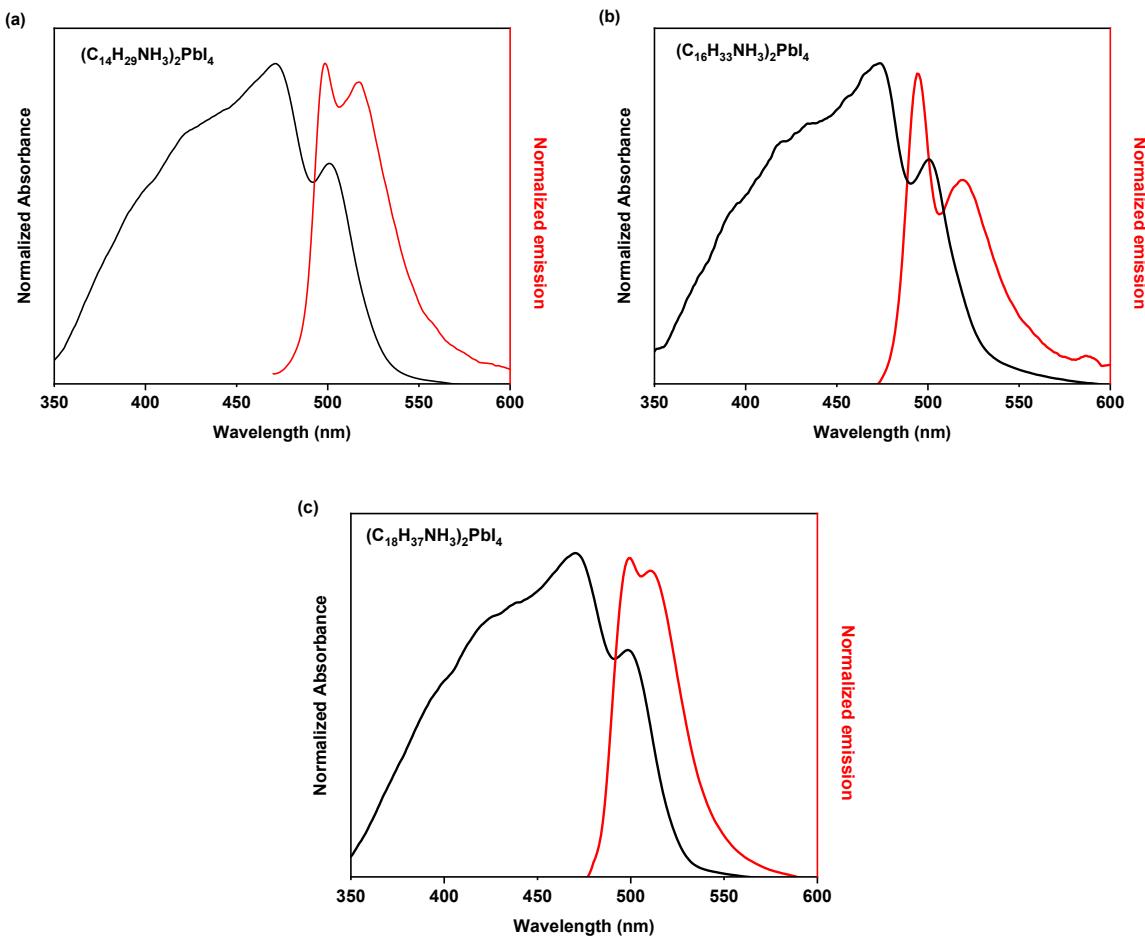
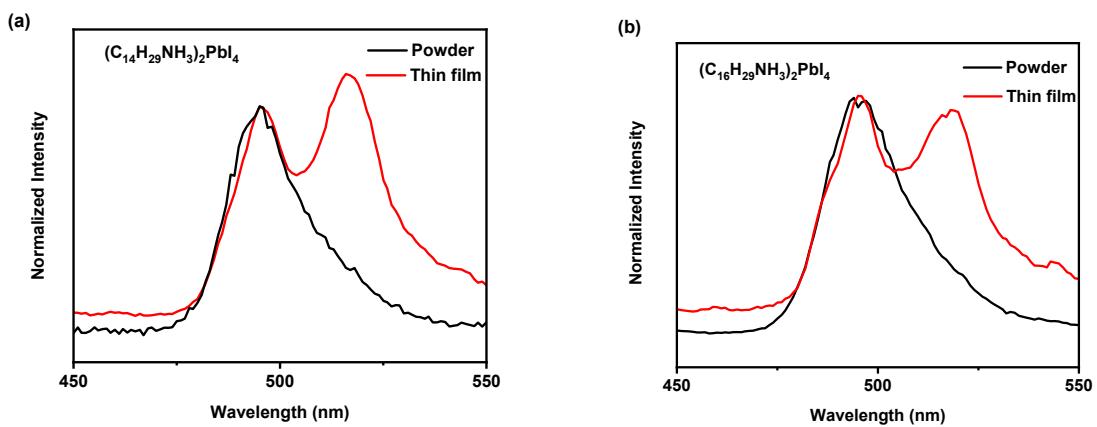


Figure S1. Absorbance and PL emission spectra of powder of (a) $(\text{C}_{14}\text{H}_{29}\text{NH}_3)_2\text{PbI}_4$, (b) $(\text{C}_{16}\text{H}_{33}\text{NH}_3)_2\text{PbI}_4$, and (c) $(\text{C}_{18}\text{H}_{37}\text{NH}_3)_2\text{PbI}_4$ at room temperature.



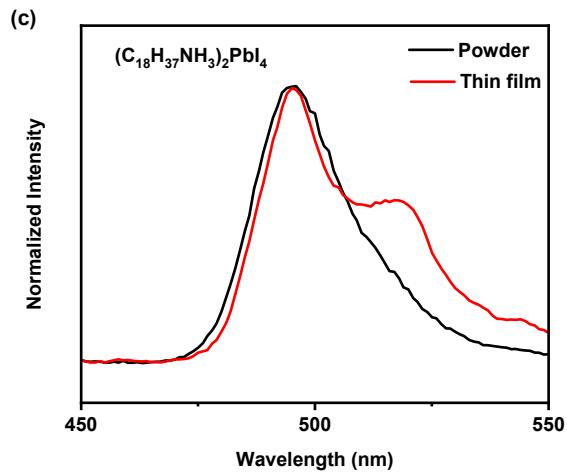


Figure S2. Comparison of PL emission spectra of (a) $(\text{C}_{14}\text{H}_{29}\text{NH}_3)_2\text{PbI}_4$, (b) $(\text{C}_{16}\text{H}_{33}\text{NH}_3)_2\text{PbI}_4$, and (c) $(\text{C}_{18}\text{H}_{37}\text{NH}_3)_2\text{PbI}_4$ thin films and fresh powder samples at room temperature.

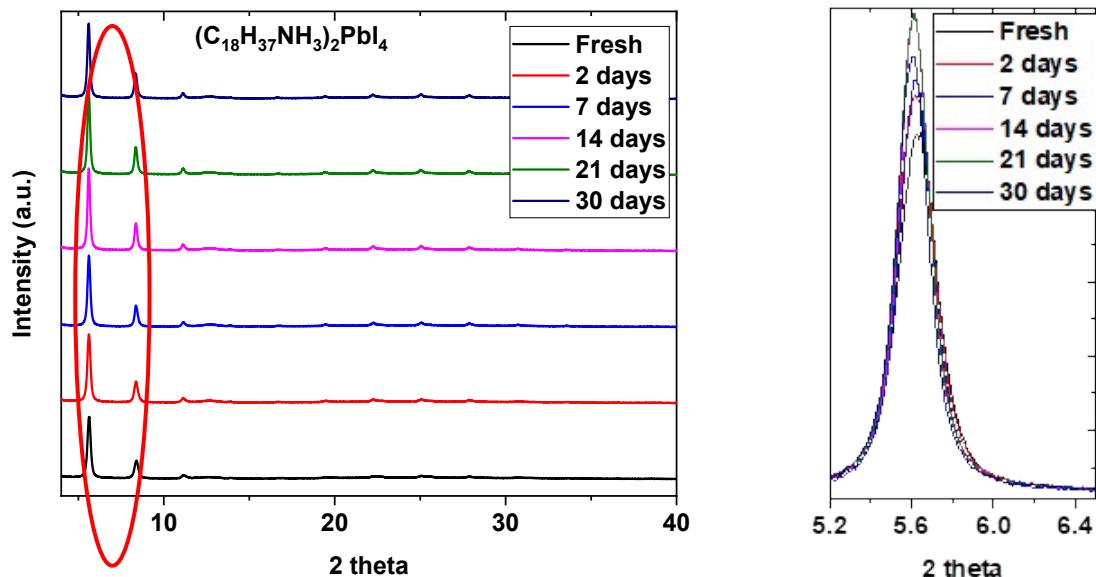


Figure S3. XRD pattern of $(\text{C}_{18}\text{H}_{37}\text{NH}_3)_2\text{PbI}_4$ 2D perovskite stored under ambient conditions.

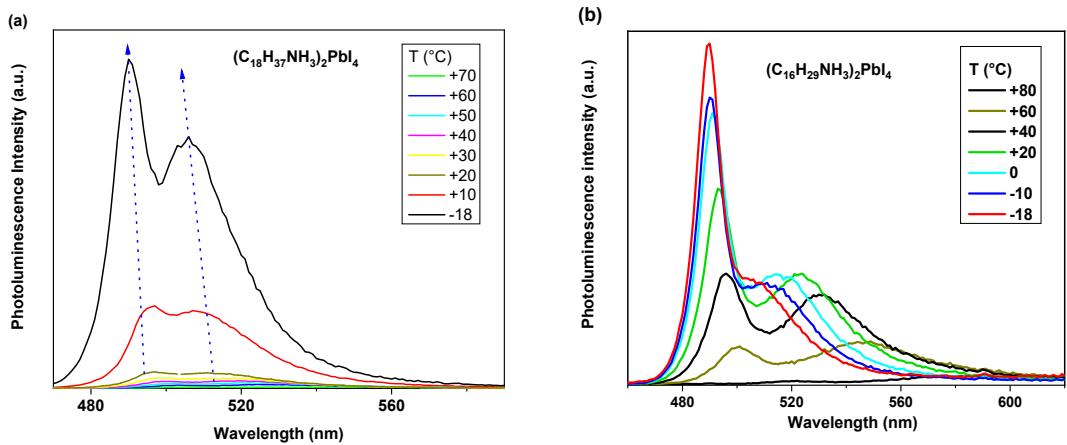


Figure S4. Temperature dependent photoluminescence spectra of (a) $(\text{C}_{18}\text{H}_{37}\text{NH}_3)_2\text{PbI}_4$, and (b) $(\text{C}_{16}\text{H}_{29}\text{NH}_3)_2\text{PbI}_4$, in the temperature range from 70 to -18°C (reverse measurement) with $\lambda_{\text{ex}} 360$ nm.

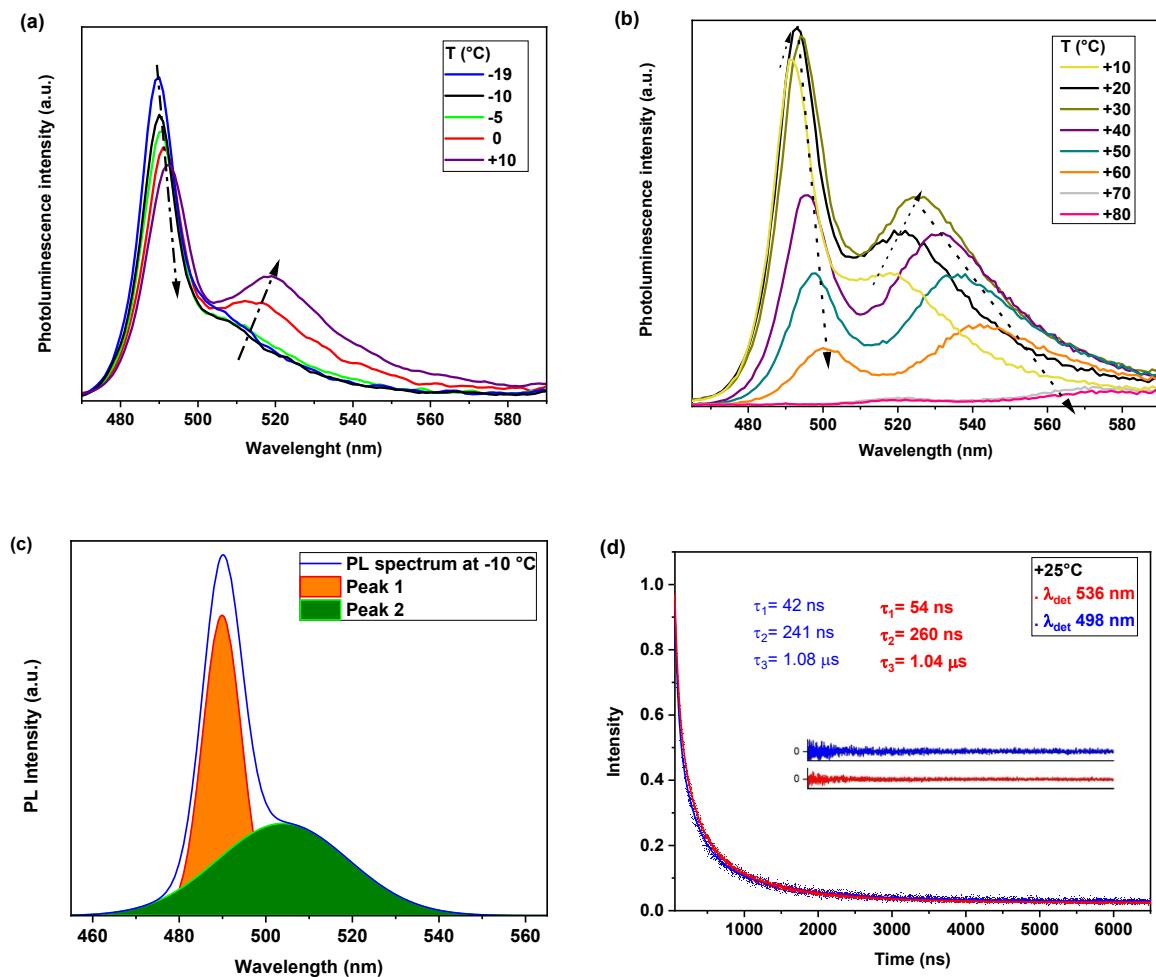


Figure S5. Temperature dependent photoluminescence spectra of $(C_{16}H_{33}NH_3)_2PbI_4$ in the temperature range (a) from -18 to 10 °C, (b) from 10 to 80 °C with λ_{ex} 360 nm. (c) Fitting of PL spectra with Gaussian multi-peak function at -10 °C. (d) Normalized time-resolved photoluminescence decay traces of $(C_{16}H_{33}NH_3)_2PbI_4$ at 25 °C.

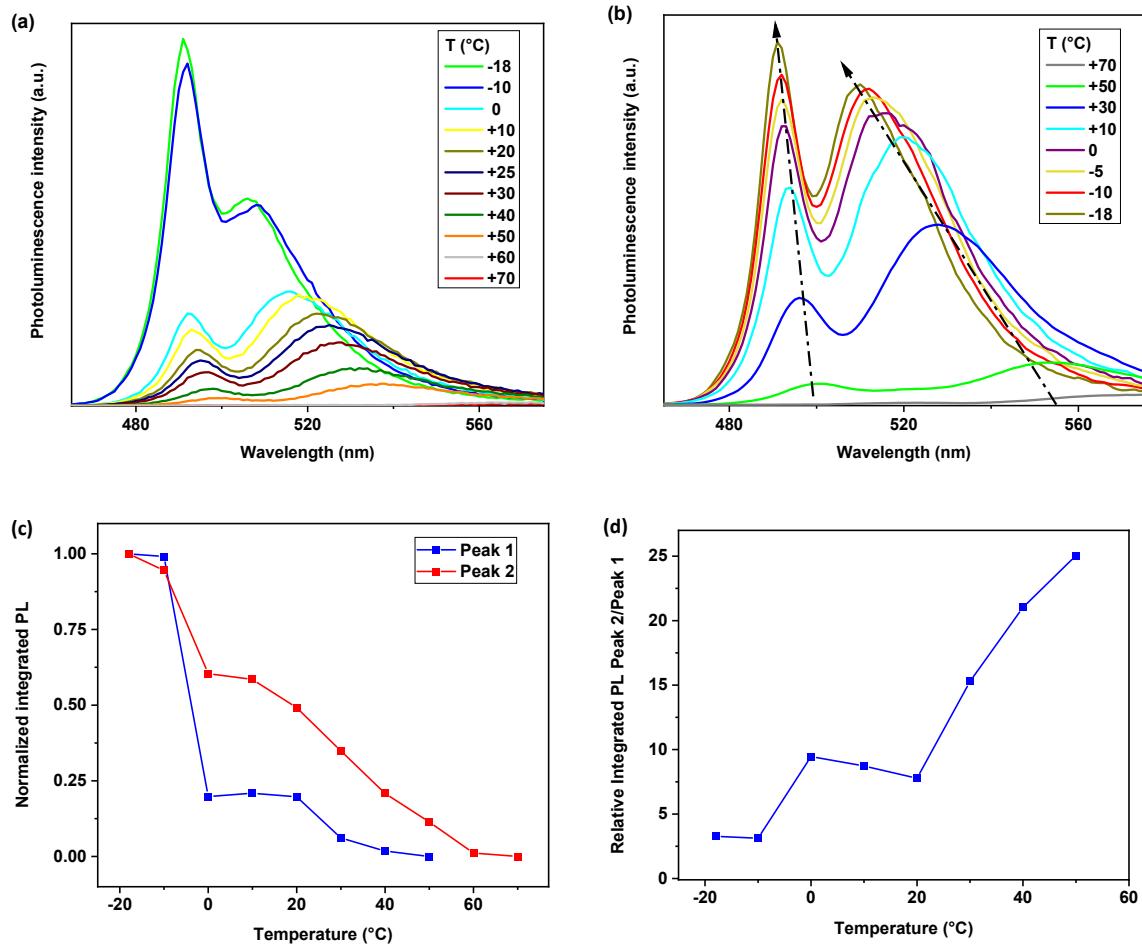


Figure S6. Temperature dependent photoluminescence spectra of $(C_{14}H_{29}NH_3)_2PbI_4$ in the temperature range from (a) -18 to 70 °C, and (b) 70 to -18 °C (reverse). (c) Variation of integrated PL intensity emission peak maxima of $(C_{14}H_{29}NH_3)_2PbI_4$. (d) Relative integrated intensities of comparing the ratio of the low energy (Peak 2) to high energy (Peak 1).

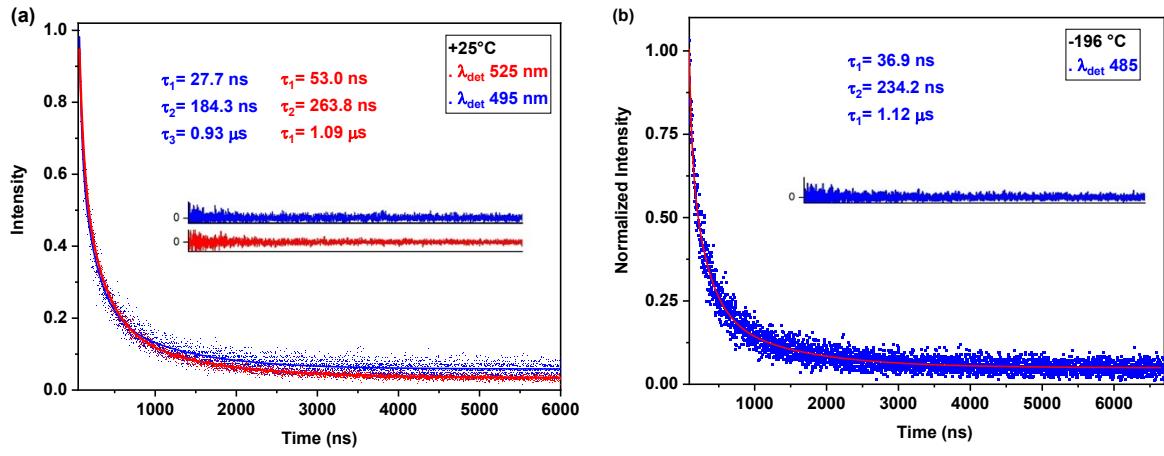


Figure S7. (a) Normalized time-resolved photoluminescence decay traces of $(\text{C}_{14}\text{H}_{29}\text{NH}_3)_2\text{PbI}_4$ powders at room temperature with $\lambda_{\text{ex}} = 360 \text{ nm}$. (b) Normalized time-resolved photoluminescence decay trace of $(\text{C}_{14}\text{H}_{29}\text{NH}_3)_2\text{PbI}_4$ powders at $-196 \text{ }^{\circ}\text{C}$ with $\lambda_{\text{ex}} = 360 \text{ nm}$.

Table S1. Quantum yield of 2D compounds at different temperatures ($^{\circ}\text{C}$) with relative method compared to room temperature.

Compound	Temperature ($^{\circ}\text{C}$)											
	-18	-10	0	10	20	30	40	50	60	70	80	85
$(\text{C}_{18}\text{H}_{37}\text{NH}_3)_2\text{PbI}_4$	6.30	3.06	2.83	3.07	2.93	2.57	1.85	1.21	0.74	0.42	0.10	0.06
$(\text{C}_{16}\text{H}_{33}\text{NH}_3)_2\text{PbI}_4$	0.14	0.07	0.13	0.18	0.23	0.28	0.21	0.17	0.10	0.023	0.018	
$(\text{C}_{14}\text{H}_{29}\text{NH}_3)_2\text{PbI}_4$	3.54	3.52	1.85	1.85	1.61	0.73	0.72	0.44	0.09	0.07		

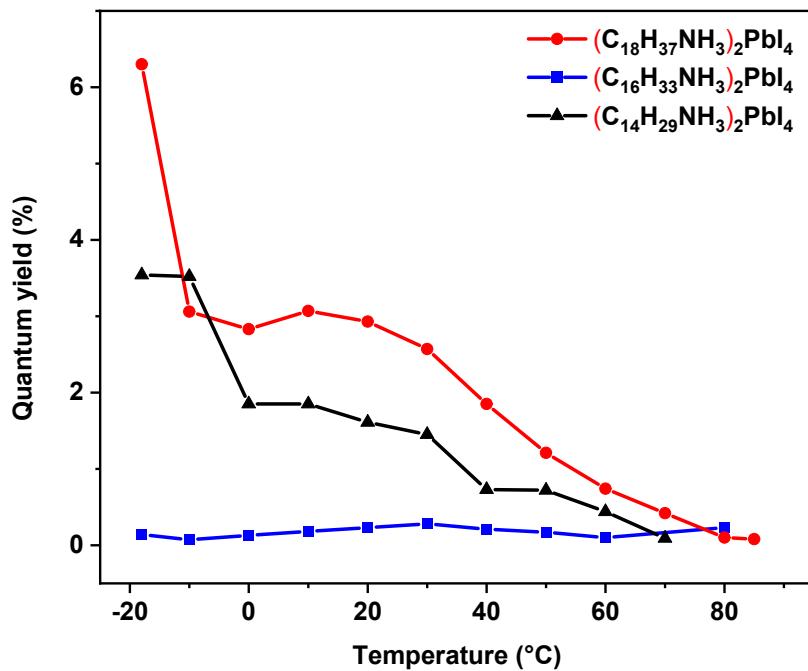


Figure S8. Temperature dependance of photoluminescence quantum yields for 2D perovskite compounds: $(C_{18}H_{37}NH_3)_2PbI_4$, $(C_{16}H_{33}NH_3)_2PbI_4$, and $(C_{14}H_{29}NH_3)_2PbI_4$.