

## Supporting Information (SI)

### Neural Networks for Analysis of Optical Properties in 2D Layered Hybrid Lead Halide Perovskites

Rayan Chakraborty,<sup>\*,‡</sup> Tariq Sheikh,<sup>‡</sup> Prasenjit Ghosh,<sup>‡,¶</sup> Angshuman Nag<sup>\*,‡</sup>

<sup>‡</sup>Department of Chemistry, Indian Institute of Science Education and Research (IISER),  
Pune, 411008, India

<sup>¶</sup>Department of Physics, and Department of Energy Sciences, Indian Institute of Science  
Education and Research (IISER), Pune, 411008, India

\*Corresponding author

Email: RC: [rayan.chakraborty@students.iiserpune.ac.in](mailto:rayan.chakraborty@students.iiserpune.ac.in) ; AN: [angshuman@iiserpune.ac.in](mailto:angshuman@iiserpune.ac.in)

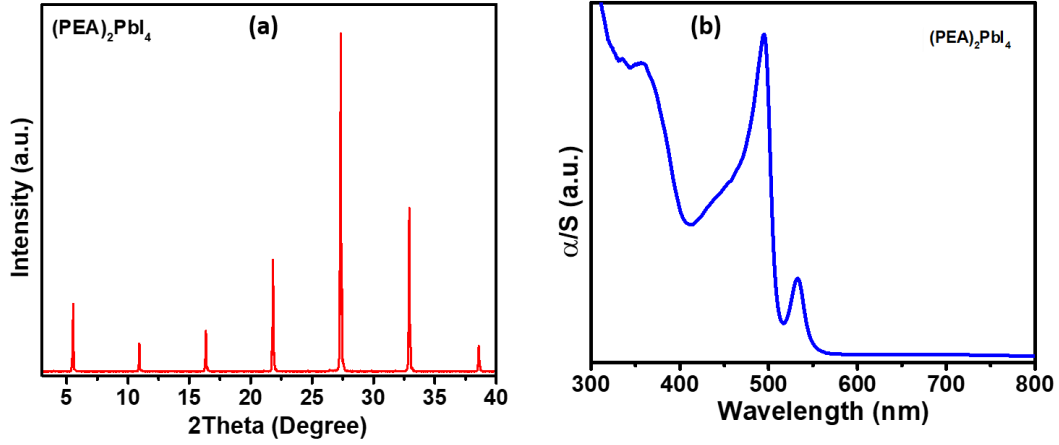


Figure S1: Characterization of (PEA)<sub>2</sub>PbI<sub>4</sub> single crystals. (a) PXRD data showing peaks corresponding to (00l) planes. (b) UV-visible absorption spectrum showing the excitonic resonance at 523 nm.  $\alpha$  is the absorption coefficient and  $S$  is the scattering coefficient. The experimental data are measured in the diffused reflectance mode and then converted to absorption data.

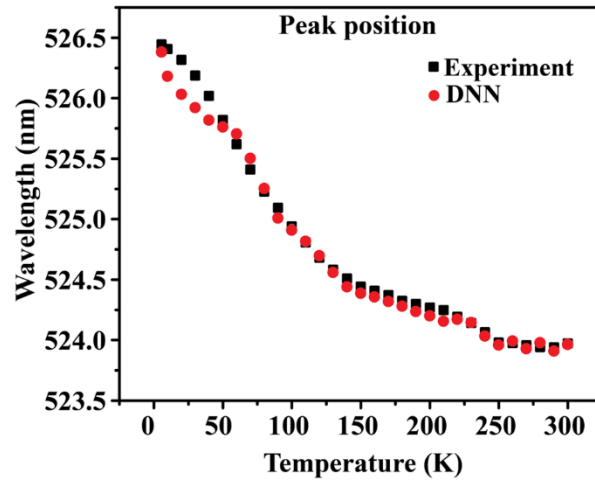


Figure S2: Variation of the excitonic emission peak with temperature in experimental and DNN-generated datasets for (PEA)<sub>2</sub>PbI<sub>4</sub> single crystals.

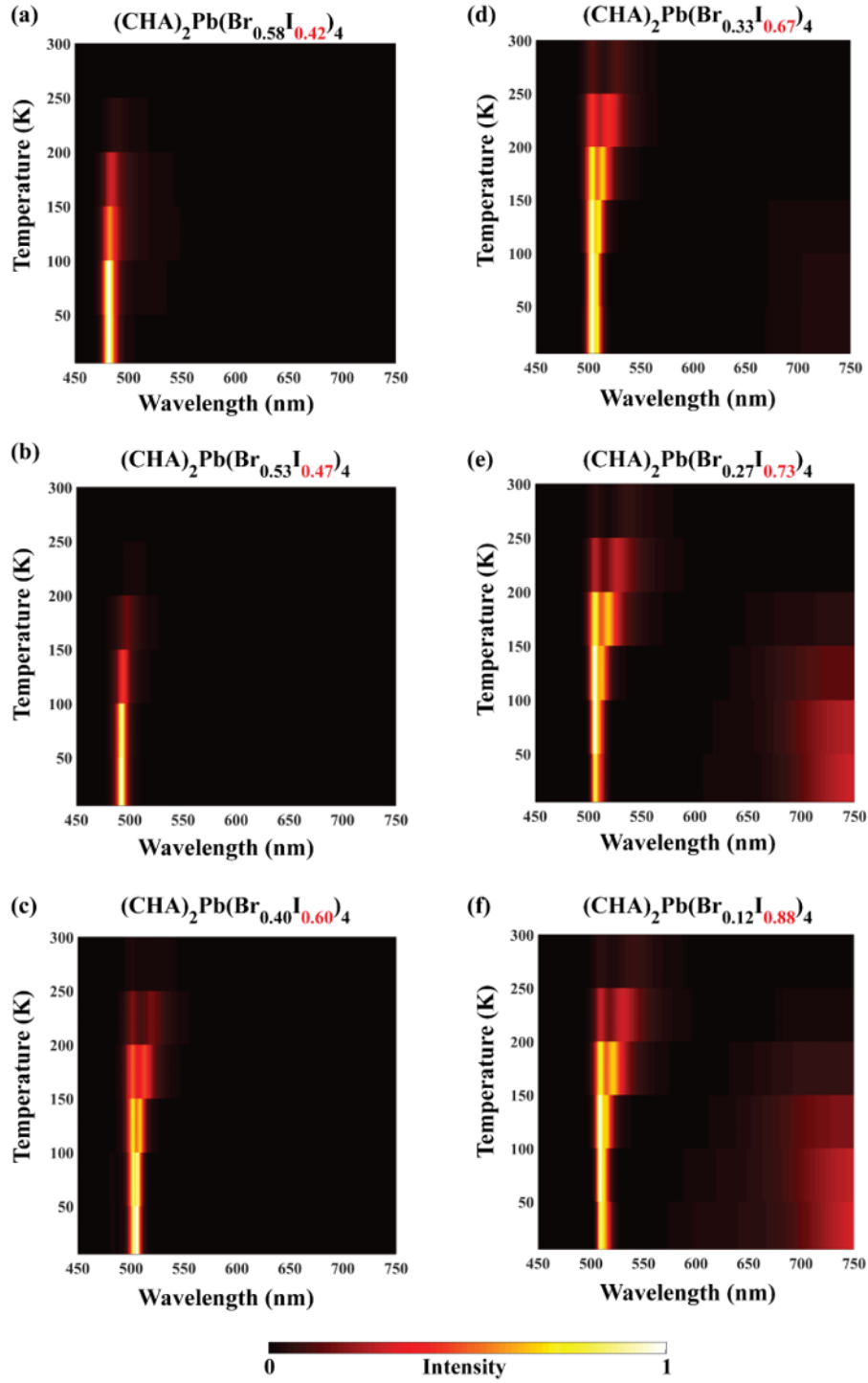


Figure S3: (a-f) Colormap generated from experimentally measured PL spectra measured at seven different temperatures (5.6, 50, 100, 150, 200, 250, and 300 K) for  $(\text{CHA})_2\text{Pb}(\text{Br}_{1-x}\text{I}_x)_4$  single crystals with different compositions “x”.

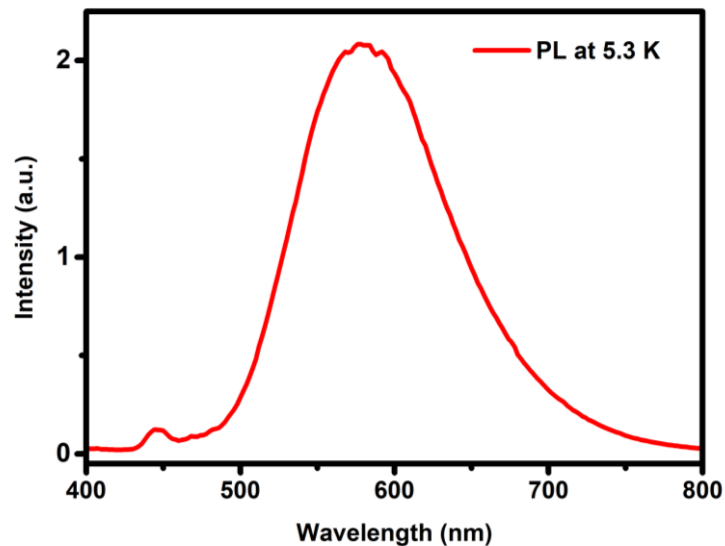


Figure S4: Photoluminescence spectrum of  $(\text{CHA})_2\text{Pb}(\text{Br}_{0.82}\text{I}_{0.18})_4$  single crystal at 5.3 K.

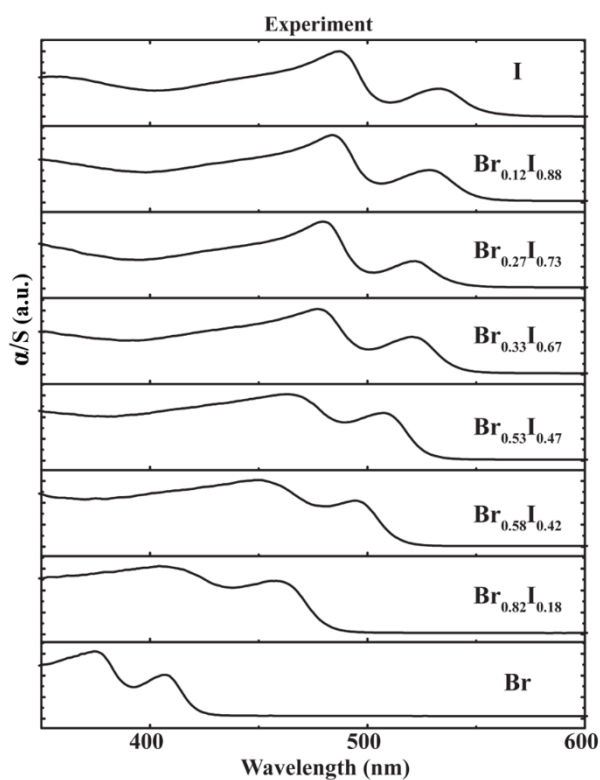


Figure S5: UV-visible absorption spectra of  $(\text{CHA})_2\text{Pb}(\text{Br}_{1-x}\text{I}_x)_4$  single crystals. The absorption spectra are obtained from the measured diffused reflectance spectra. Here,  $\alpha$  is the absorption coefficient and  $S$  is the scattering coefficient.