

## Supporting Information

### **Stable Self-Trapped Broadband Emission from an Organolead Halide Coordination Polymer with Strong Layer Corrugation and High Chemical Robustness**

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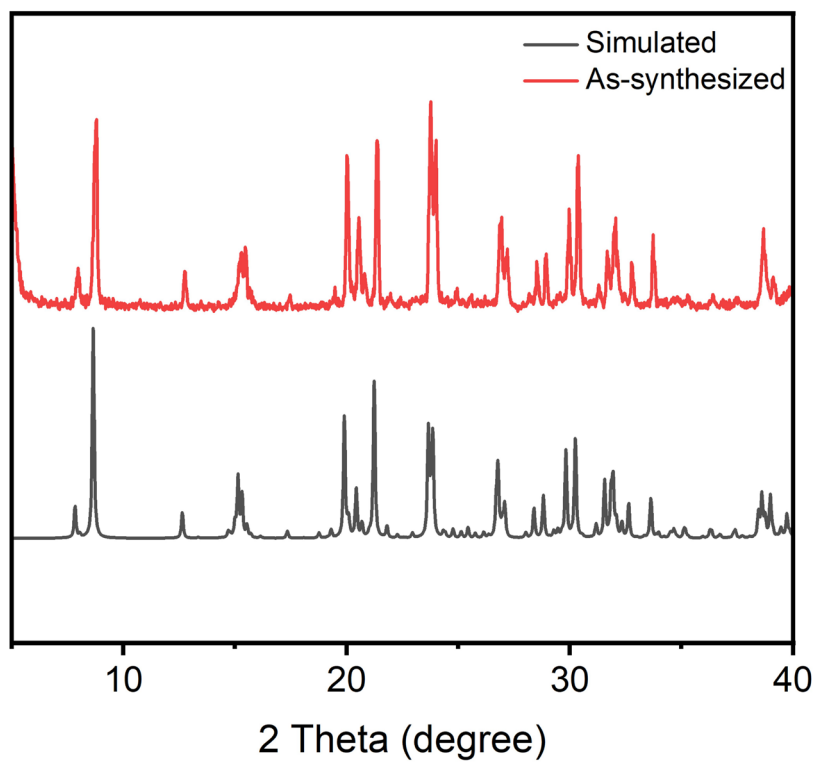
**Table S1.** Crystallographic data and structure refinement for TJU-19.

|  |   |
|--|---|
| Identification code  | TJU-19  |
| Empirical formula  | Pb <sub>2</sub> Cl <sub>2</sub> C <sub>5</sub> H <sub>2</sub> N <sub>2</sub> O <sub>4</sub> |
| Formula weight   | 639.37  |
| Temperature/K  | 297.0   |
| Crystal system   | triclinic   |
| Space group  | <i>P</i> -1   |
| <i>a</i> /Å  | 7.0068(8)   |
| <i>b</i> /Å  | 12.0274(16)   |
| <i>c</i> /Å  | 12.3700(15)   |
| $\alpha$ /°  | 65.906(4)   |
| $\beta$ /°   | 89.857(4)   |
| $\gamma$ /°  | 87.582(4)   |
| <i>V</i> /Å <sup>3</sup>   | 950.7(2)  |
| <i>Z</i>   | 4   |
| $\rho_{\text{calc}}$ /cm <sup>3</sup>  | 4.467   |
| $\mu$ /mm <sup>-1</sup>  | 35.926  |
| <i>F</i> (000)   | 1104.0  |
| Crystal size/mm <sup>3</sup>   | 0.12 × 0.11 × 0.11  |
| Radiation  | MoK $\alpha$ ( $\lambda$ = 0.71073)   |
| 2 $\theta$ range for data collection/°   | 5.82 to 55.04   |
| Index ranges   | -9 ≤ <i>h</i> ≤ 8, -15 ≤ <i>k</i> ≤ 15, -16 ≤ <i>l</i> ≤ 15                                 |
| Reflections collected  | 22509   |
| Independent reflections  | 4369 [ <i>R</i> <sub>int</sub> = 0.0666, <i>R</i> <sub>sigma</sub> = 0.0511]                |
| Data/restraints/parameters   | 4369/0/271  |
| Goodness-of-fit on <i>F</i> <sup>2</sup>   | 1.119   |
| Final <i>R</i> indexes [ <i>I</i> ≥ 2 $\sigma$ ( <i>I</i> )]   | <i>R</i> <sub>1</sub> = 0.0343, <i>wR</i> <sub>2</sub> = 0.0648                             |
| Final <i>R</i> indexes [all data]  | <i>R</i> <sub>1</sub> = 0.0531, <i>wR</i> <sub>2</sub> = 0.0707                             |
| Largest diff. peak/hole / e Å <sup>-3</sup>  | 1.50/-2.03  |
| $R_1 = \sum( F_o  -  F_c ) / \sum F_o $ ; $wR_2 = \{\sum[w(F_o^2 - F_c^2)] / \sum[w(F_o^2)]\}^{1/2}$ |   |

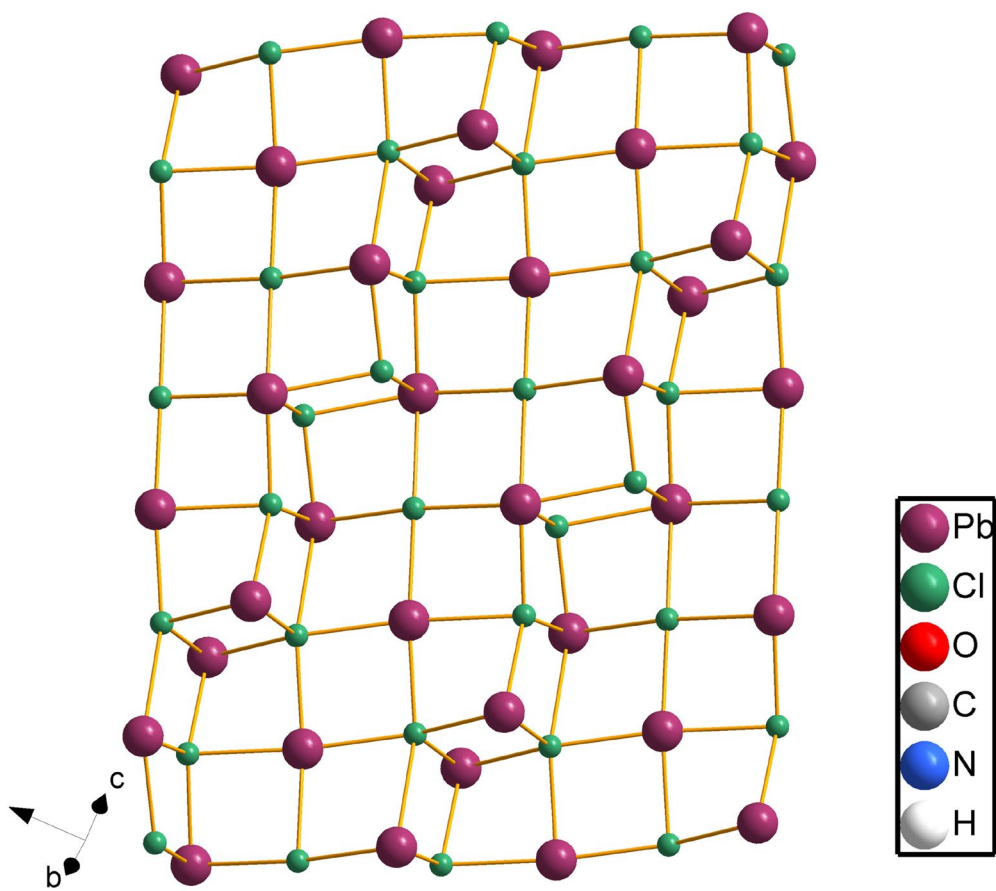
**Table S2.** Photophysical properties of TJU-19

| Material | $\lambda_{\text{abs}}$ <sup>a</sup> | $\lambda_{\text{em}}$ <sup>b</sup> | ( <i>x</i> , <i>y</i> ) <sup>c</sup> | PLQY <sup>d</sup> |
|----------|-------------------------------------|------------------------------------|--------------------------------------|-------------------|
| TJU-19   | 347 nm                              | 520 nm                             | (0.23, 0.45)                         | 12.9%             |

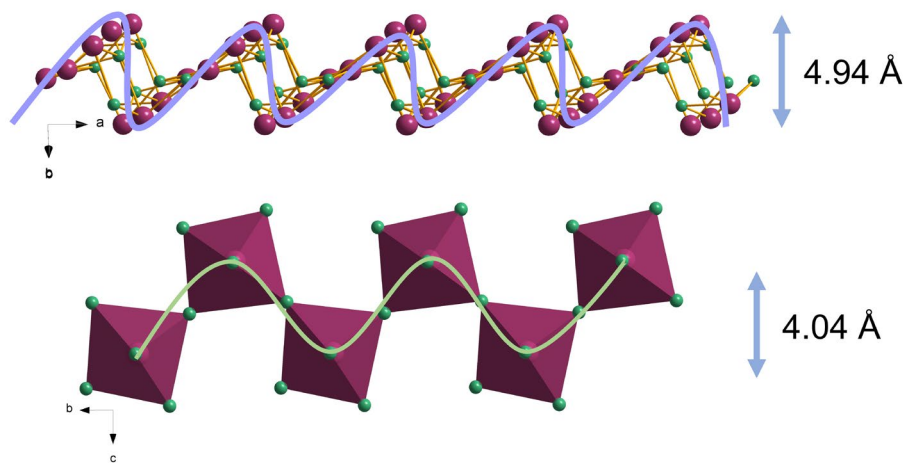
<sup>a</sup>  $\lambda_{\text{abs}}$  is the absorption edge; <sup>b</sup>  $\lambda_{\text{em}}$  is the maximum emission wavelength; <sup>c</sup> (*x*, *y*) is the chromatic coordinates; <sup>d</sup> PLQY is photoluminescence quantum yield.



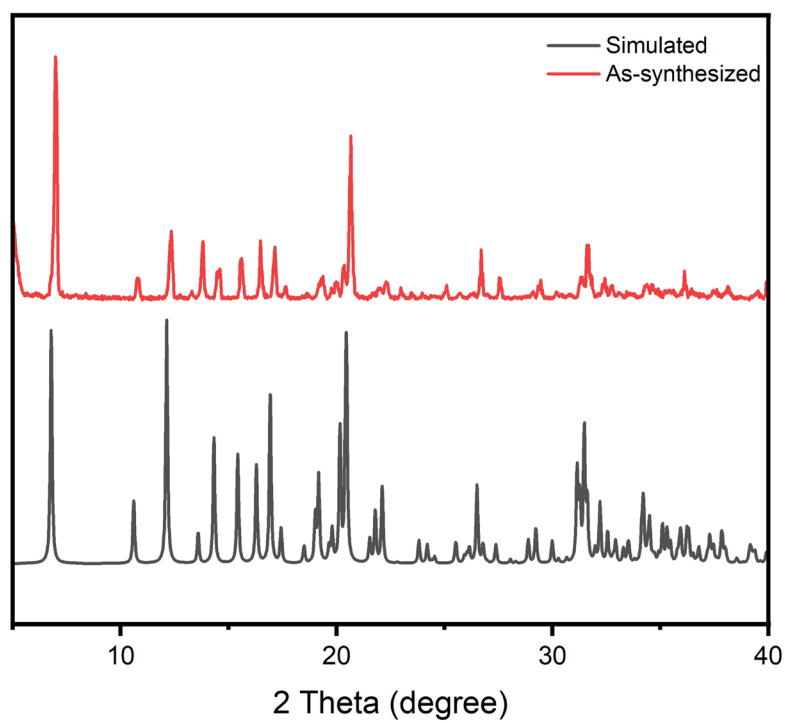
**Figure S1.** Simulated and experimental PXRD of TJU-19.



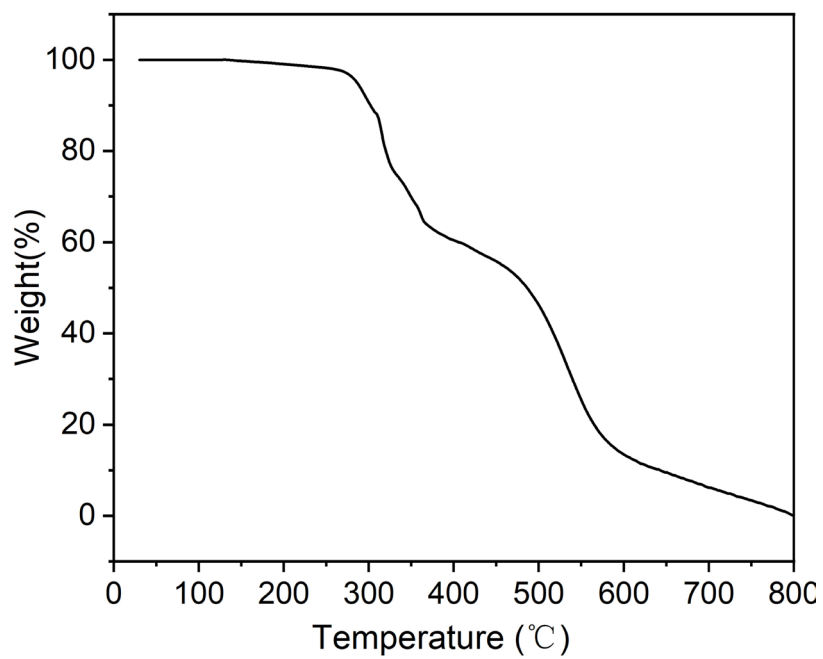
**Figure S2.** Crystallographic top-view of a single  $[\text{Pb}_2\text{Cl}_2]^{2+}$  layer.



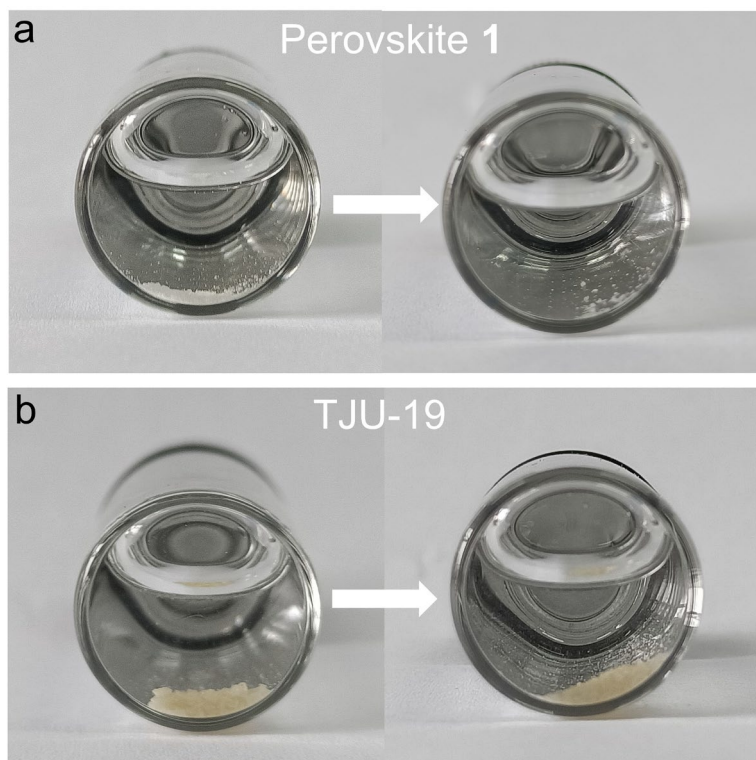
**Figure S3.** Layer corrugation of a single  $[\text{Pb}_2\text{Cl}_2]^{2+}$  layer of TJU-19 and a single layer of (110)-oriented perovskite 1.



**Figure S4.** Simulated and experimental PXRD of perovskite **1**.



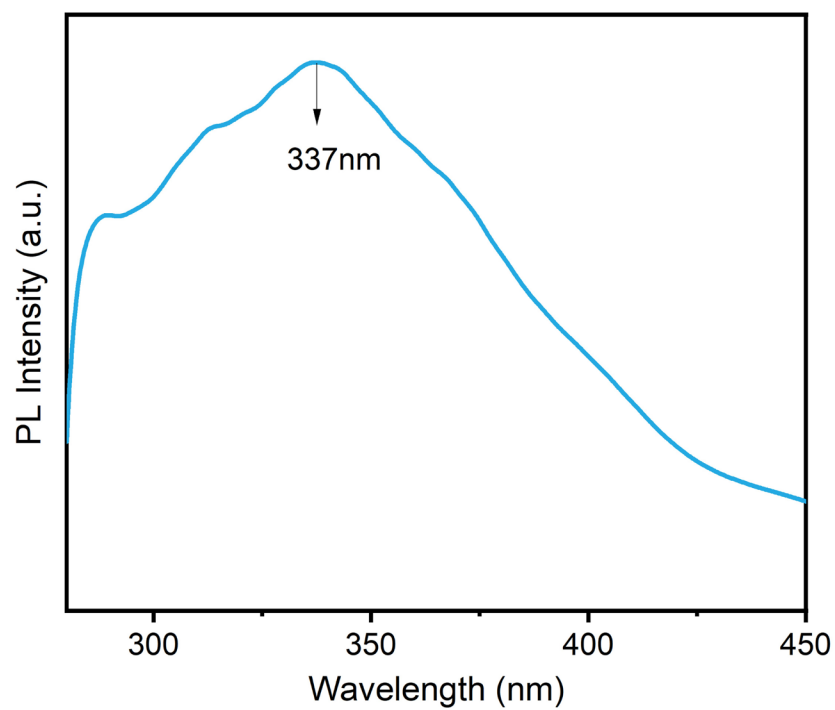
**Figure S5.** Thermogravimetric analysis of TJU-19 in N<sub>2</sub> flow.



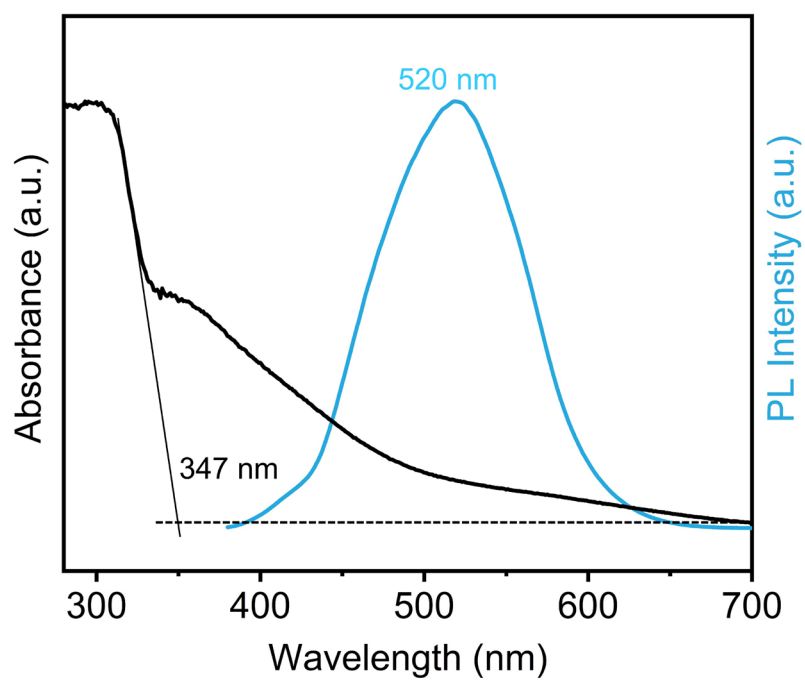
**Figure S6.** Photographs of perovskite **1** and TJU-19 in pure water before and after 24

h.

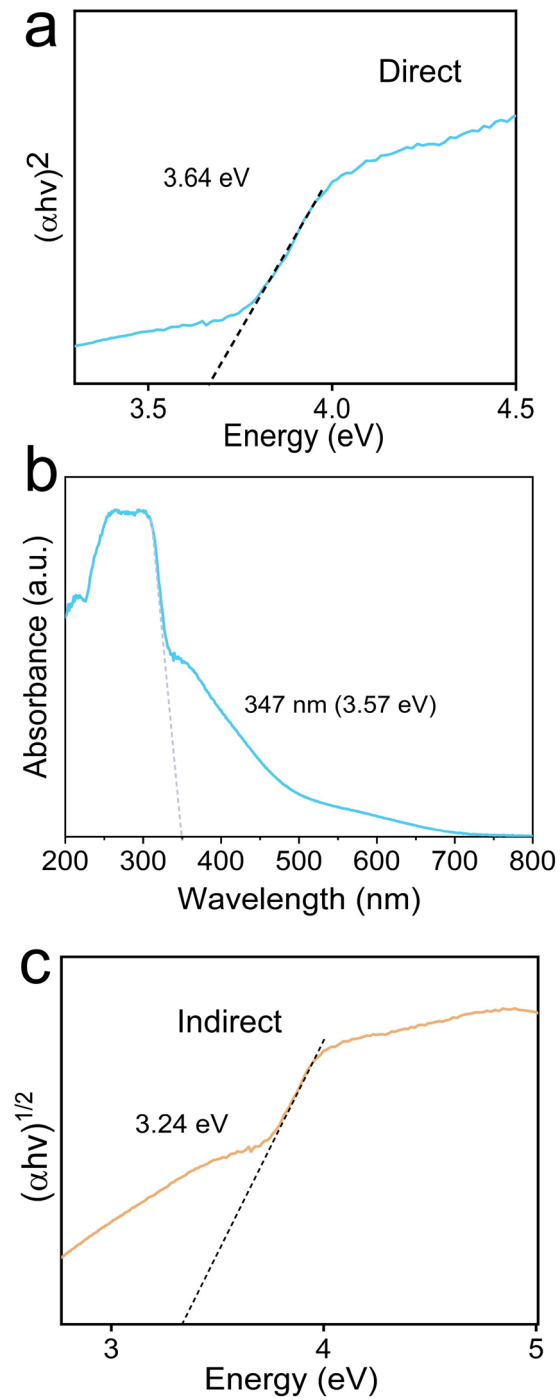




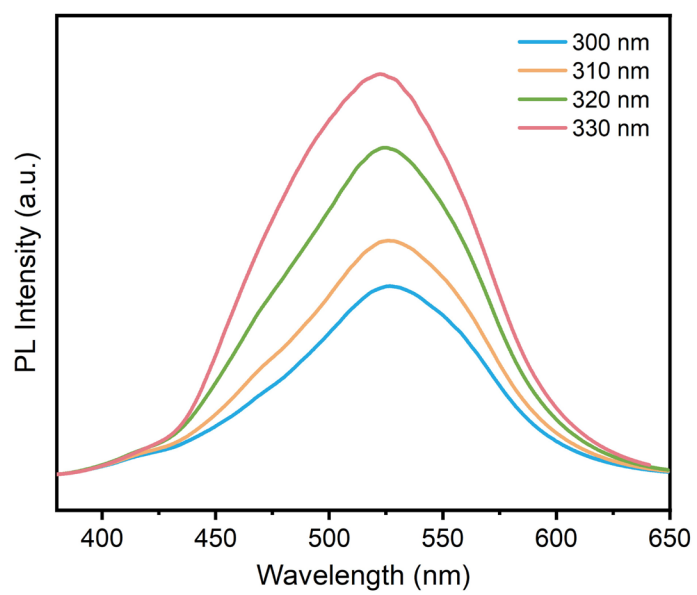
**Figure S7.** Excitation spectra of TJU-19 at room temperature.



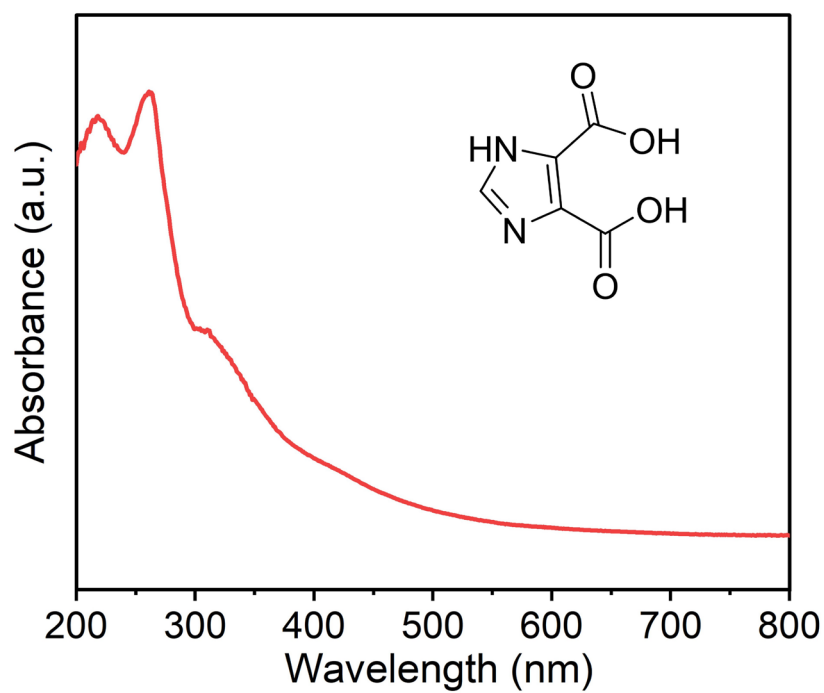
**Figure S8.** UV-vis diffuse reflectance spectroscopy and photoluminescence spectra of TJU-19 measured at room temperature.



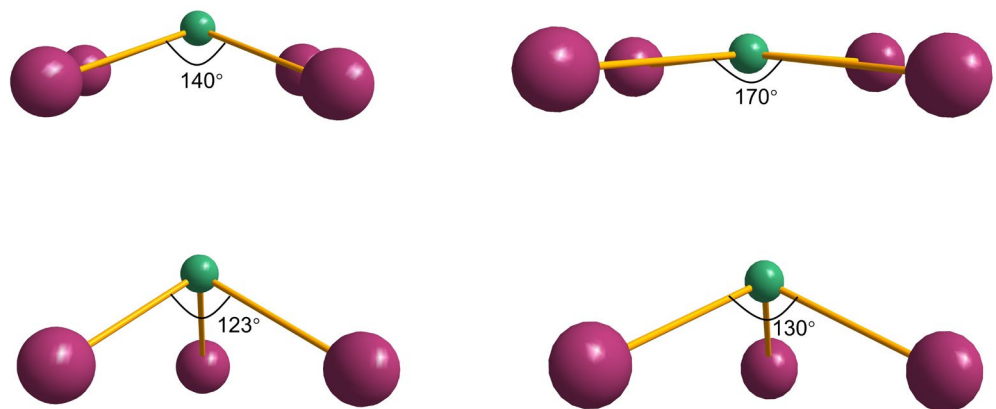
**Figure S9.** (a) Tauc plot of TJU-19 fitted by direct bandgap. (b) UV-vis diffuse reflectance spectroscopy of TJU-19. (c) Tauc plot of TJU-19 fitted by indirect bandgap.



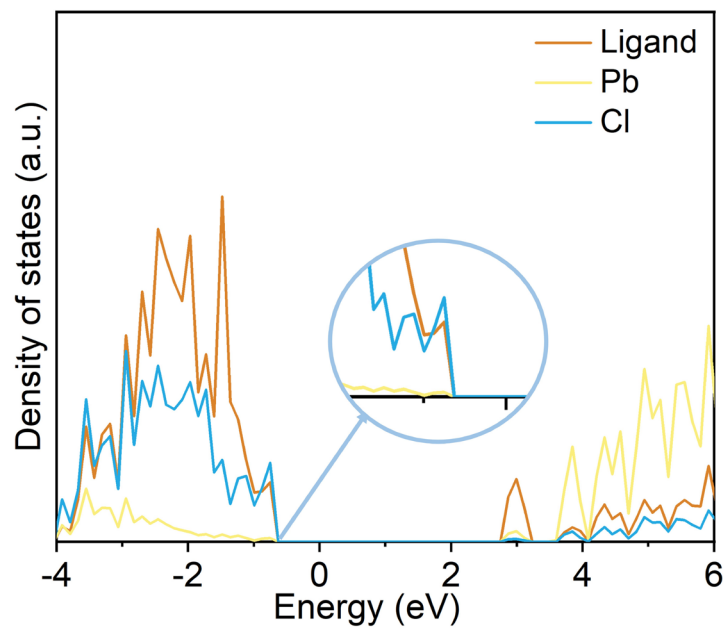
**Figure S10.** Excitation-dependent emission spectra of TJU-19 from 300 to 330 nm.



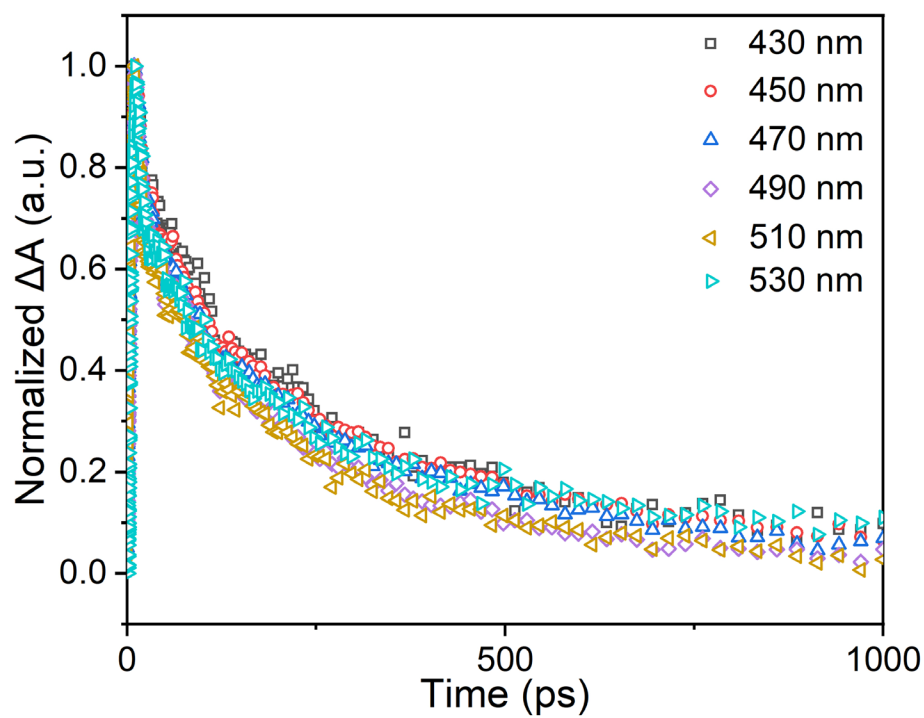
**Figure S11.** UV-vis absorption spectra of the free imdc<sup>2-</sup> ligands.



**Figure S12.** The coordination environment of the  $\mu_3/\mu_4$ -bridging chloride species in TJU-19.

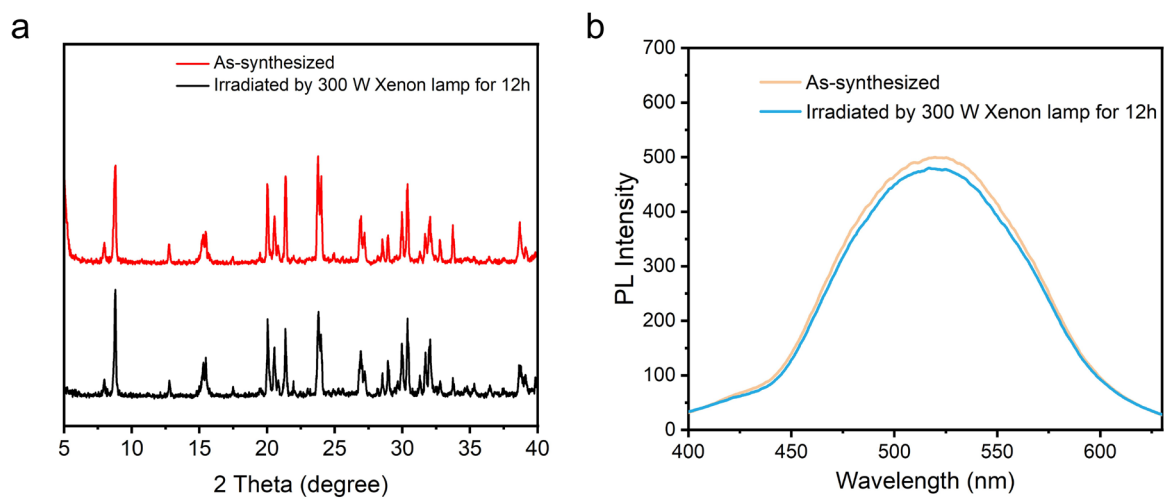


**Figure S13.** Calculated DOS for the ligand (orange), Cl (blue) and Pb (yellow) in TJU-19.



**Figure S14.** TA kinetics of TJU-19 ranging from 400 to 550 nm.





**Figure S15.** PXRD and emission spectra of TJU-19 before and after continuous illumination in air from a 300 W Xe lamp for 12 h.