

Supporting information

Antimony based organic-inorganic hybrid coating material with high quantum efficiency and thermal quenching effect

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Materials. SbCl₃ (99.9% metals basis), 1-carboxymethyl-3-methylimidazolium chloride (98%) acetonitrile (>99%), ethylacetate (AR, 99%) were purchased from Aladdin. All reagents and solvents were used without further purification unless otherwise stated.

Single crystal synthesis of 1. A mixture of SbCl₃ (0.0228 g, 0.1 mmol), 1-carboxymethyl-3-methylimidazolium chloride (0.0354 g, 0.2 mmol) in acetonitrile (6 mL) and ethylacetate (2 mL) was stirred in a 20 mL glass bottle for 1 hour to form a white precipitate. The mixture was then sealed in a Teflon-lined bomb and heated to a temperature of 120 °C for 3 days and cooled slowly to room temperature. Colorless crystals and white polycrystalline powder were slowly precipitated out from the solution. Upon completion of the reaction, powder sample of **1** was collected by filtration from the reaction solution and washed with a small amount of acetonitrile for three times. The sample was then dried in a vacuum oven overnight before other measurements were made.

Single crystal X-ray diffraction (SXRD). Single crystal X-ray diffraction data were collected at 173 K on a Bruker D8 Venture diffractometer with graphite-monochromated Ga K α radiation ($\lambda = 1.34139 \text{ \AA}$) The structure was solved by direct methods and refined by full-matrix least-squares on F² using the Bruker SHELXTL package. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif. The structure was deposited in Cambridge Structural Database (CSD) and the number is 1960644.

Powder X-ray diffraction (PXRD). PXRD analyses were carried out on a Bruker D8 Advance automated diffraction system using Cu K α radiation ($\lambda=1.5406 \text{ \AA}$). The data were collected at room temperature in a 2θ range of 3-50° with a scan speed of 1°/min.

The operating power was 40 kV/40 mA.

Optical diffuse reflectance measurements. Optical diffuse reflectance spectra were measured at room temperature on a Shimadzu UV-3600 spectrophotometer. Data were collected in the wavelength range of 300-1200 nm. BaSO₄ powder was used as a standard (100% reflectance). A similar procedure as previously described was used to collect and convert the data using the Kubelka-Munk function. The scattering coefficient (S) was treated as a constant since the average particle size of the samples used in the measurements was significantly larger than 5 μm.

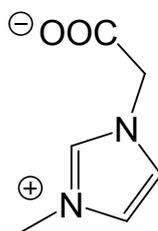
Thermogravimetric (TG) analysis. TG analysis of the title compound was performed on a computer-controlled TG 550 (TA Instrument). Pure powder sample was loaded into platinum pans and heated with a ramp rate of 10 °C/min from room temperature to 700 °C.

Excitation spectrum measurements. Excitation spectra were measured at room temperature on a FLS1000 spectrofluorometer (Edinburgh Instruments) monitored at maximum of emission spectra.

Photoluminescence measurements. Steady-state photoluminescence spectra were obtained at room temperature and 77 K (liquid nitrogen was used to cool the samples) on a FLS1000 spectrofluorometer.

Internal quantum yield measurements. Internal quantum yield (IQY) of the sample in powder form was measured on a C9920-03 absolute quantum yield measurement system (Hamamatsu Photonics) with a 150 W xenon monochromatic light source and 3.3 inch integrating sphere.

Time-resolved photoluminescence. Time-Resolved Emission data were collected at room temperature using the FLS1000 spectrofluorometer. The dynamics of emission decay were monitored by using the FLS1000's time-correlated single-photon counting capability (1024 channels; 10 μs window) with data collection for 10,000 counts. Excitation was provided by an Edinburgh EPL-360 picosecond pulsed diode laser. Long lifetime measurements at 77K (1024 channels; 800 μs window) were collected using Xe flash lamp as the excitation source. The lifetime was obtained by mono-exponential fitting.



2-(3-methyl-1*H*-imidazol-3-ium-1-yl)acetate

Figure S1. Structural plot of the organic ligand.

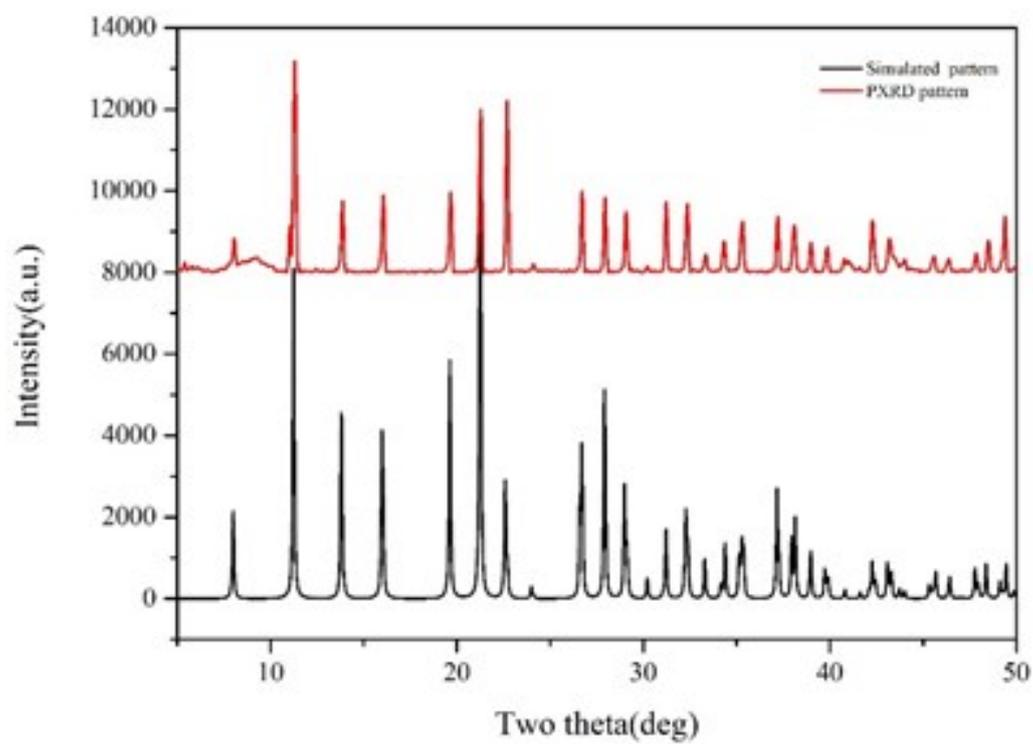


Figure S2. PXRD patterns of the as-made (top) and simulated pattern (bottom) of compound 1.

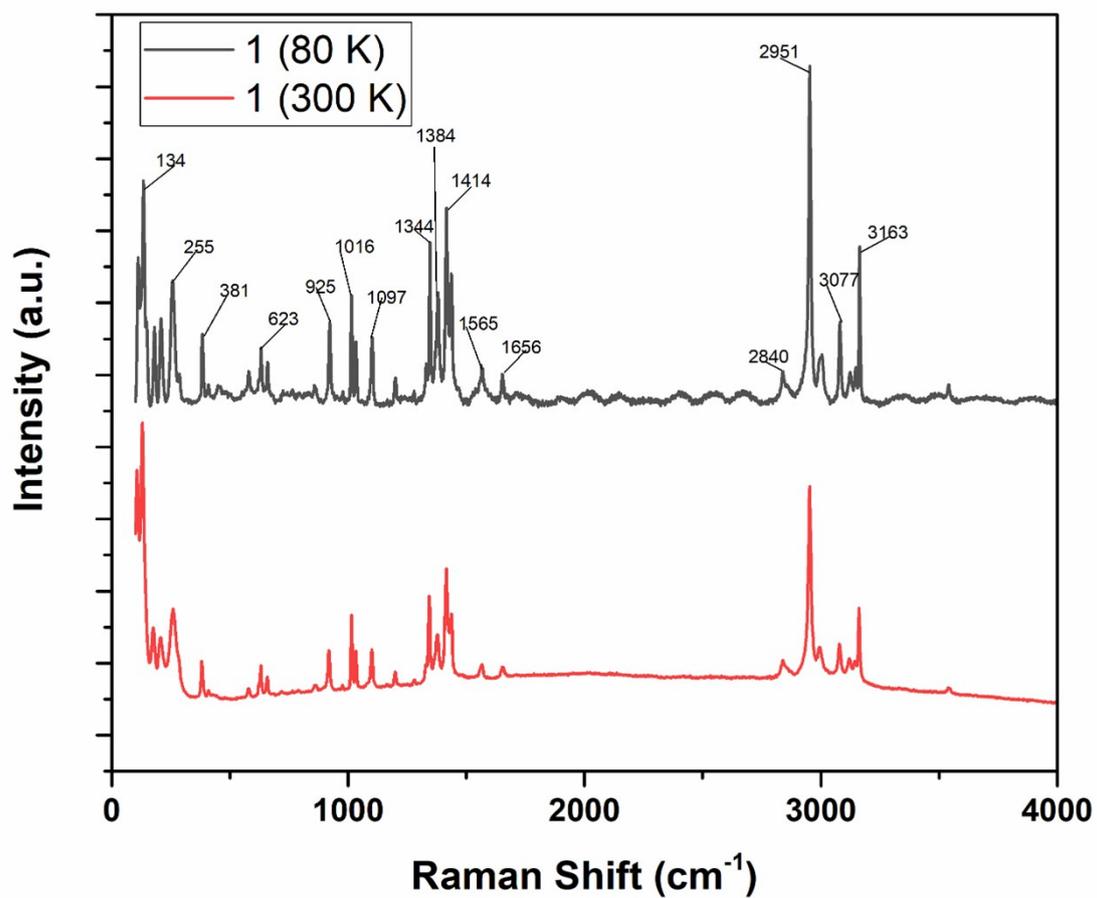


Figure S2a. Raman spectra of compound **1** at 300 K and 80 K.

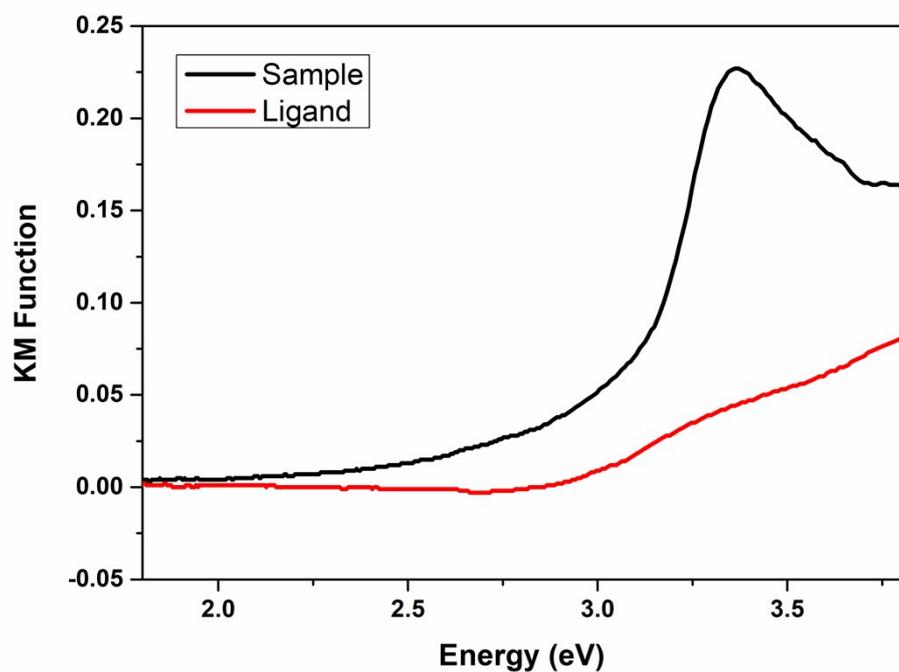


Figure S3. Optical absorption spectrum of compound **1** and ligand.

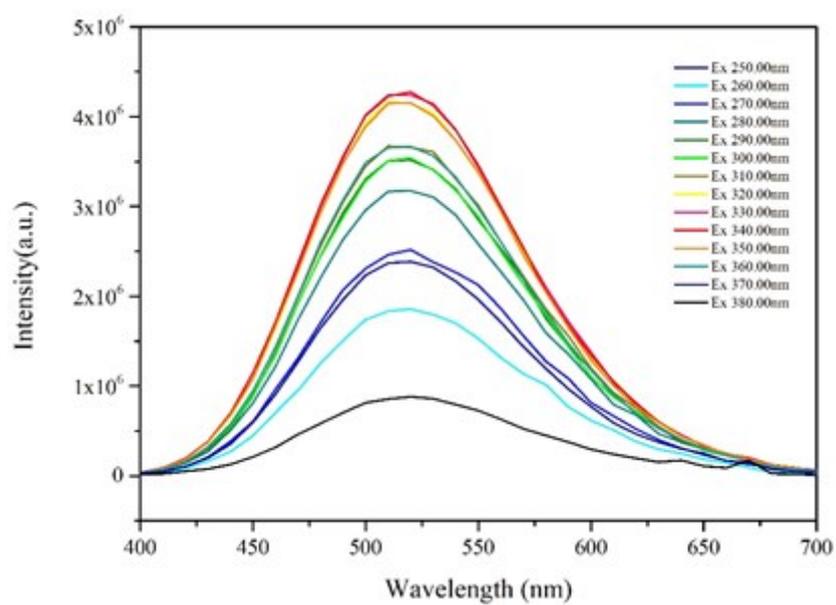


Figure S4. Emission spectra of **1** under various excitation energies.

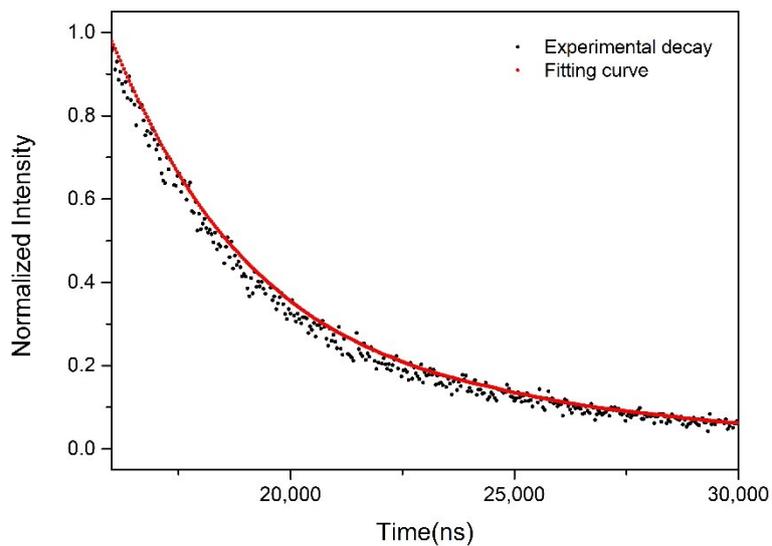


Figure S5. Luminescence decay curve of compound **1** at room temperature.

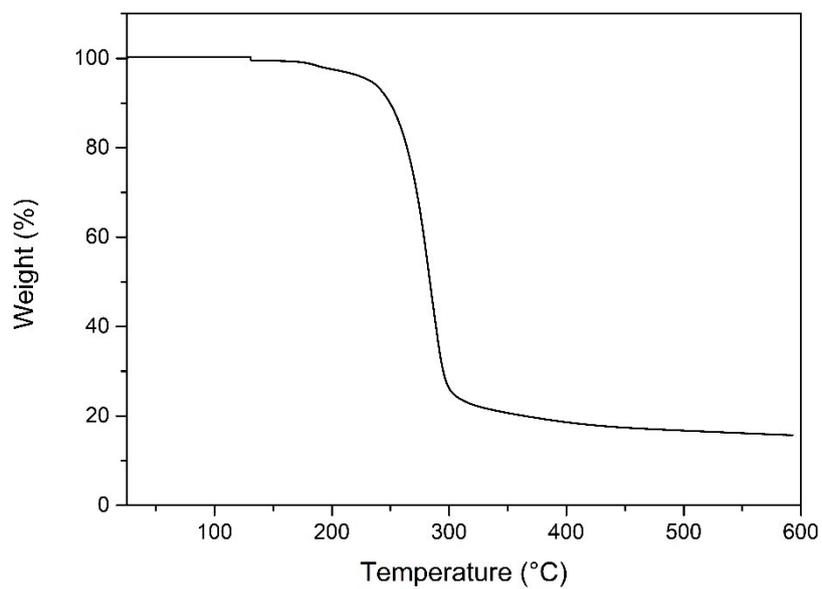


Figure S6. TGA plot of compound **1**.

Table S1. Single crystal X-ray diffraction data of compound **1**

Compound	1
Formula	$C_{36}H_{54}Cl_6N_{12}O_{12}Sb$

Fw	1181.36
Space Group	R3
a (Å)	22.0964 (5)
b (Å)	22.0964 (5)
c (Å)	8.6309 (2)
α (°)	90
β (°)	90
γ (°)	120
V (Å ³)	3649.47 (19)
Z	3
T (K)	173 (2)
λ (Å)	1.34139
ρ (g·cm ⁻³)	1.613
Rwp	0.1892
Rp	0.0648