Supporting Information

D-π-A type tetraphenylethylene-based AIEgen: multi-stimuli responsive behavior and multilevel anti-counterfeiting application

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1. Materials and apparatus

All solvents and chemicals were purchased from Energy Chemical or Macklin Biochemical Co., Ltd., and were used directly as received. Tetrahydrofuran (THF) used for spectral determination was of HPLC grade, other reagents were of analytical grade. The solutions of metal ions were prepared from $Al(ClO_4)_3{\cdot}9H_2O$, $CaCl_2$, $Cd(ClO_4)_2{\cdot}H_2O$, $Co(ClO_4)_2{\cdot}6H_2O$, $CrCl_3{\cdot}6H_2O$, $FeCl_3{\cdot}6H_2O$, KCl, LiCl, $MgCl_2{\cdot}6H_2O$, $Mn(ClO_4)_2{\cdot}6H_2O$, NaCl, $Ni(ClO_4)_2{\cdot}6H_2O$, $Zn(Ac)_2$, $ZnCl_2$, $Zn(ClO_4)_2{\cdot}6H_2O$, $Zn(NO_3)_2{\cdot}6H_2O$, $Pb(ClO_4)_2{\cdot}3H_2O$, $FeCl_2$, $Cu(ClO_4)_2{\cdot}6H_2O$. ^1H NMR and ^{13}C NMR spectra were acquired on a Bruker Ascend 400 (400 MHz) spectrometer. FT-IR spectra were obtained on a Bruker INVENIO Fourier transform infrared spectrometer using KBr pellets. UV-vis absorption spectra were collected on an UV-2600 spectrophotometer. X-ray powder diffraction (PXRD) pattern was obtained using a Bruker D8 Advance diffractometer with Cu-Kα radiation (λ = 1.5418 Å) at 25 °C. Fluorescence spectra were recorded by a Thermo Scientific Lumina fluorescence spectrophotometer, with a quartz cuvette (path length = 1 cm). pH values were determined on a PHS-3E pH meter. MALDI-TOF mass spectrum was acquired on a Bruker UltrafleXtreme MALDI-TOF mass spectrometer. X-ray photoelectron spectra

(XPS) were recorded using a Thermo Scientific K-Alpha XPS spectrometer. ESI-HRMS were collected on a Thermo Scientific Q Exactive Orbitrap mass spectrometer equipped with an ESI interface.

2. Synthesis of compound 1

As shown in Figure S1, bromotriphenylethylene (0.67 g, 2 mmol) and 4-formylphenylboronic acid (0.36 g, 2.4 mmol), K_2CO_3 solution (2 mol/L, 14 mL) and 30 mL THF were mixed and stirred for 30 min at room temperature under nitrogen atmosphere. Then tetrakis(triphenylphosphine)palladium (0.15 g, 0.017 mmol) was added, and the mixture was further heated to 68 ℃ and stirred overnight. After cooling to room temperature, the reaction mixture was filtered through diatomaceous earth, and the obtained filtrate was extracted with water to obtain the organic phase, which was then dried by anhydrous $MgSO_4$. The organic phase was evaporated under reduced pressure and purified by column chromatography using dichloromethane/hexane (3/1, v/v) as eluent to obtain the yellowish powder, namely 4-(triphenylvinyl)benzaldehyde with a yield of 84%. ^{1}H NMR (400 MHz, $CDCl_3$) (**Figure S1**): δ 9.94 (s, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.18-7.14 (m, 9H), 7.08-7.03 (m, 6H).

3. Synthesis of compound 2

2-methyl-5-(4-pyridinyl)-8-quinolinol (2) was prepared according to the reported literature[1, 2]. ^{1}H NMR (400 MHz, DMSO-d_6): δ 8.71 (d, *J* = 4.0 Hz, 2H), 8.17 (d, *J* = 8.0 Hz, 1H), 7.51-7.44 (m, 4H), 7.20 (d, *J* = 8.0 Hz, 1H), 2.74 (s, 3H).

4. Single-crystal structure determination

Single-crystal diffraction data of **HL** were collected on a Bruker D8 Venture diffractometer equipped with a graphite monochromated Mo-Kα radiation (λ = 0.71073 Å) at 273 K. The structure was solved by charge-flipping algorithm and refined by full matrix least squares based on F^2 with SHELX-2018/3 program[3, 4] using the Olex2 package[5, 6].

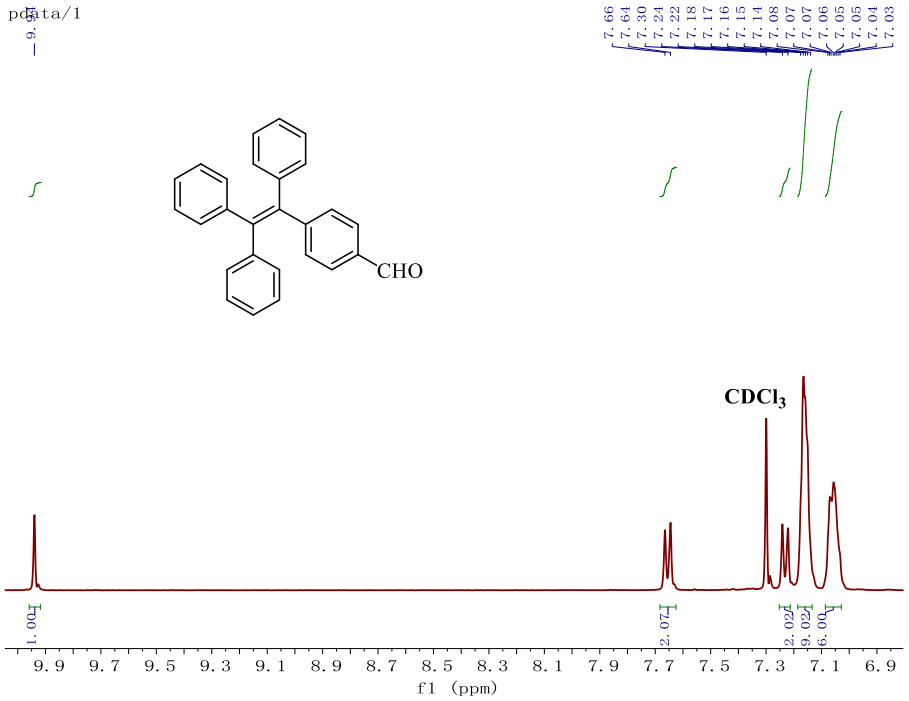
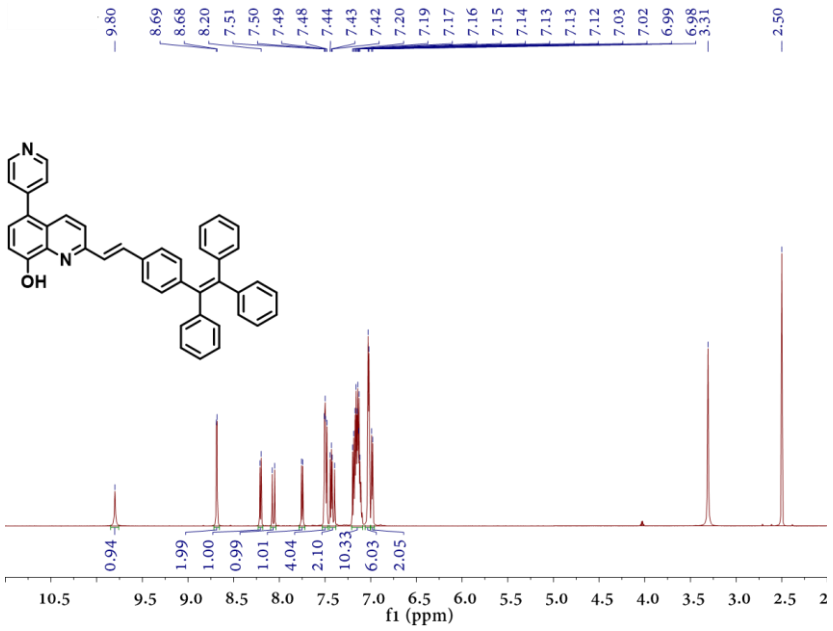


Fig. S1.[1]H NMR spectrum of compound **1** in DMSO-d_6.



(a)

Fig. S2. [1]H NMR spectrum of compound HL[2] in DMSO-d_6.

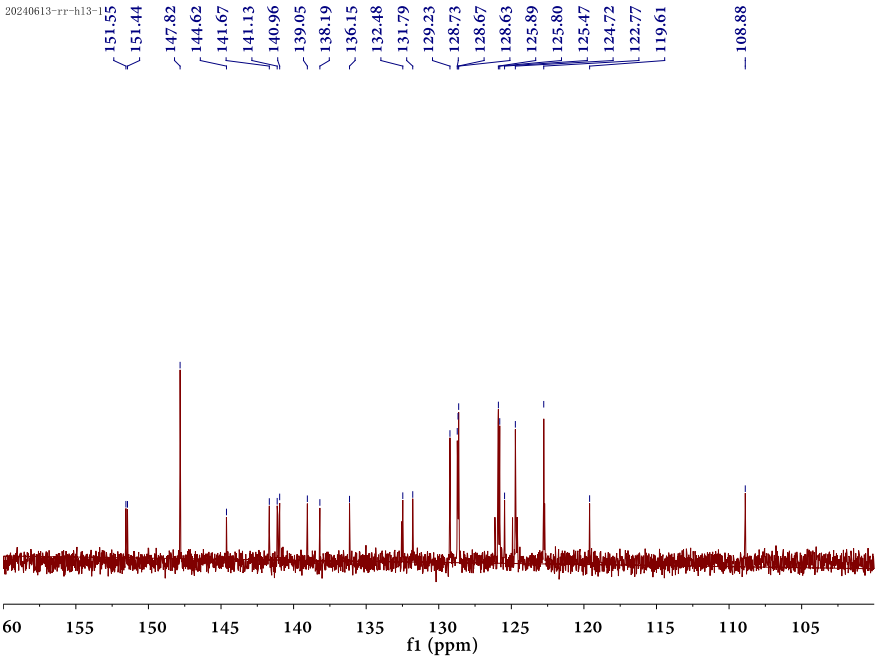


Fig. S3.^{13}C NMR spectrum of compound **HL** in DMSO-d_6.

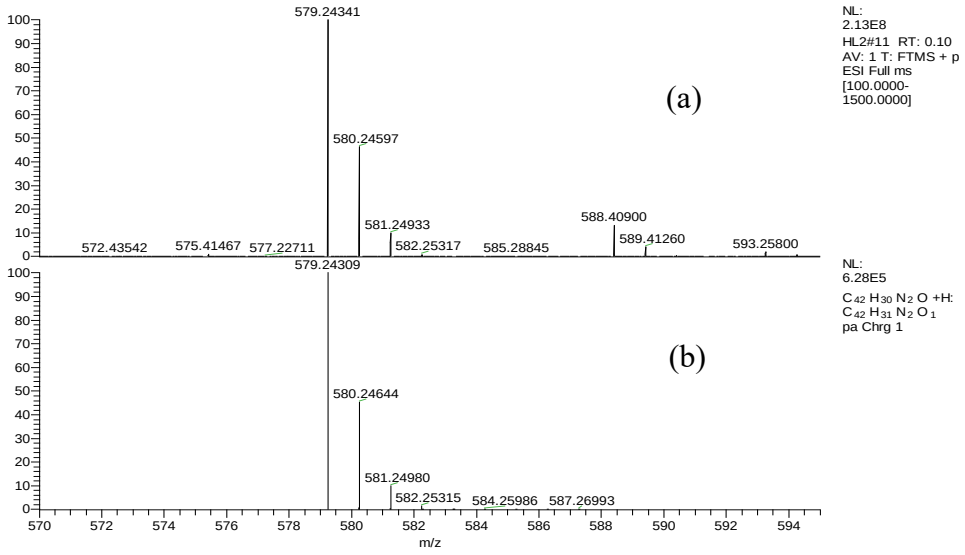


Fig. S4. (a) ESI-mass spectrum of compound HL ($C_{42}H_{30}N_2O$). (b) The simulation pattern of $[H(C_{42}H_{30}N_2O)]^+$.

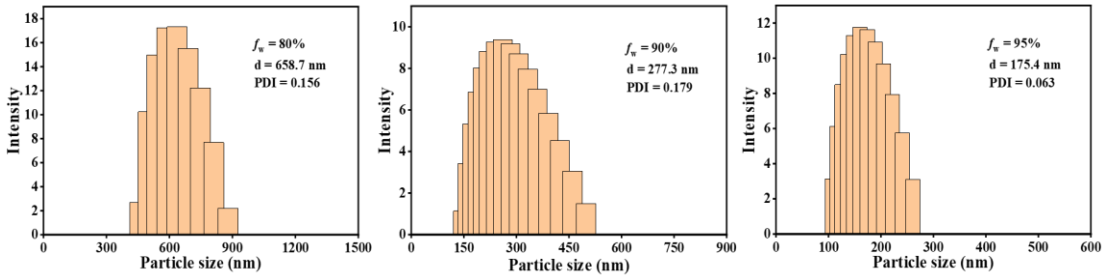


Fig. S5. DLS of HL in THF/H_2O (HEPES buffer, 20 mM, pH = 7.4) with different water fractions (f_w = 80%, f_w = 90%, f_w = 95%).

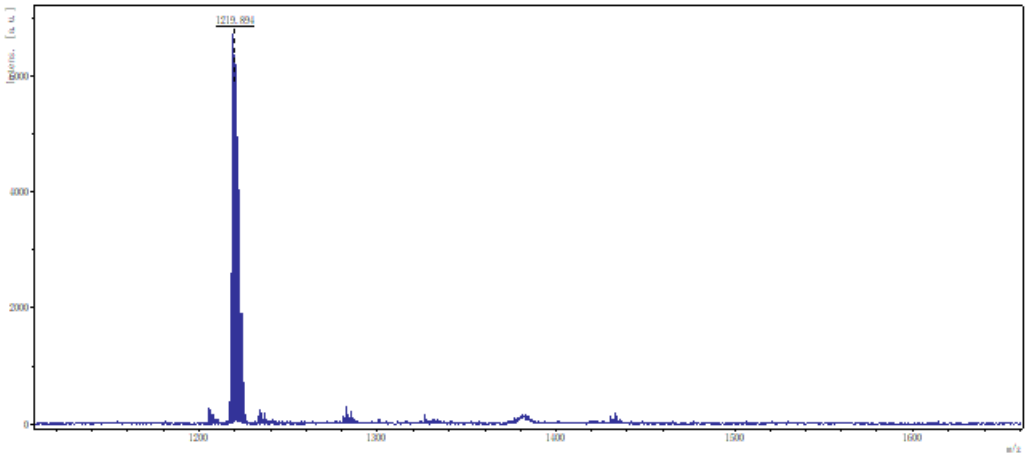


Fig. S6. Maldi-TOF-MS of HL upon the addition of 0.5 equiv. Zn^{2+} in THF.

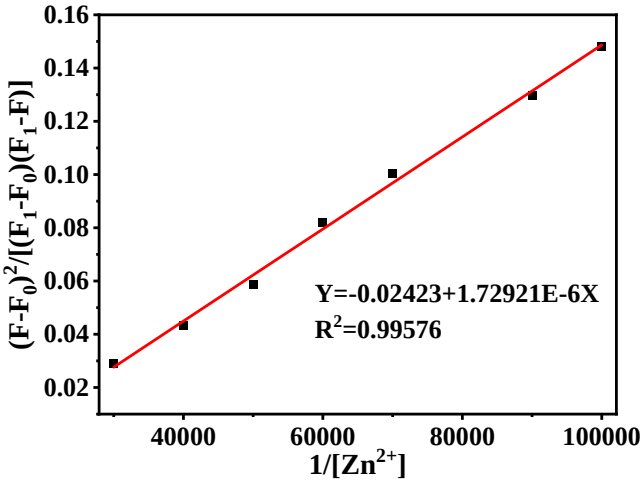


Fig. S7. Association constant calculations by plotting $(F-F_0)^2/[(F_1-F_0)(F_1-F)]$ vs $1/[Zn^{2+}]$ with linear fitting as well to find out the association constant of L^- with Zn^{2+}.

The association constant (K_a) between Zn^{2+} and L^- can be calculated on account of the following formula (1) and the linear relationship between $(F-F_0)^2/[(F_1-F_0)(F_1-F)]$ and $1/[Zn^{2+}]$ shown in Figure S7.

$$(F-F_0)^2/[(F_1-F_0)\,(F_1-F)] = 1/(2KC_L[M]) \qquad (1)$$

Where F = PL intensity at 595 nm at any given concentration of Zn^{2+}, F_0 = PL maxima in presence of Zn^{2+}, and F_1 = PL maxima in the absence of Zn^{2+}.

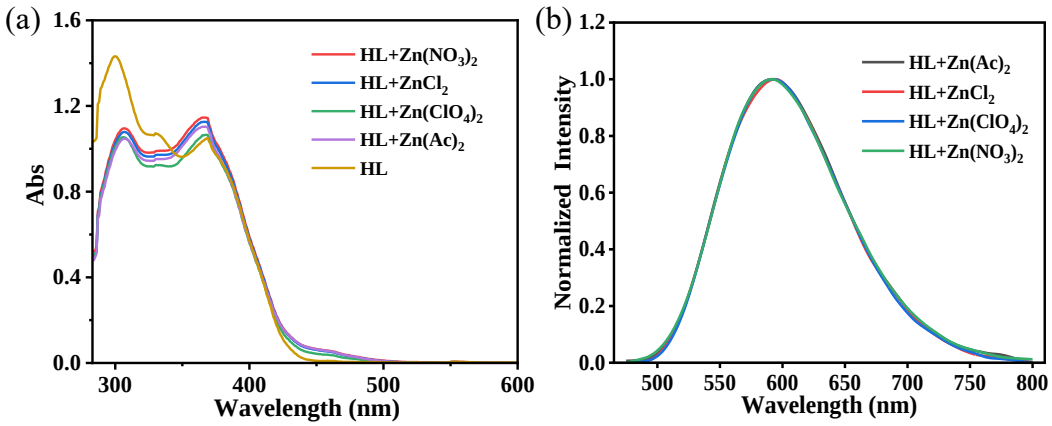


Fig. S8. UV-vis absorption spectra (a) and fluorescence spectra (b) of HL (20 μM) with 1.0 equiv. different Zn^{2+} salts stated.

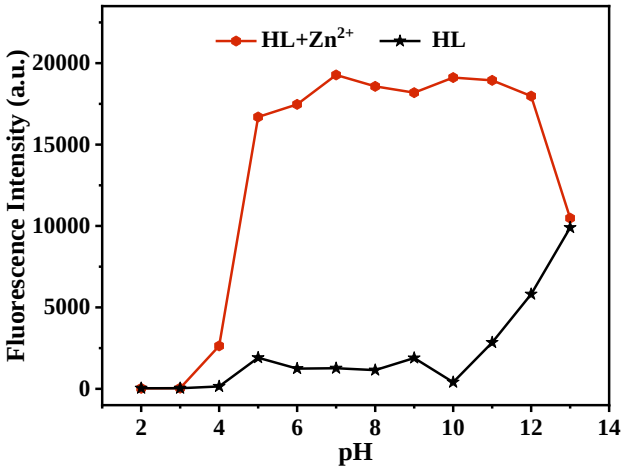


Fig. S9. Emission intensities at 595 nm of **HL** and **HL** upon addition of 0.5 equiv. Zn^{2+} in THF/H_2O (1:1, *v*/*v*) with different pH values. λ_{ex} = 465 nm.

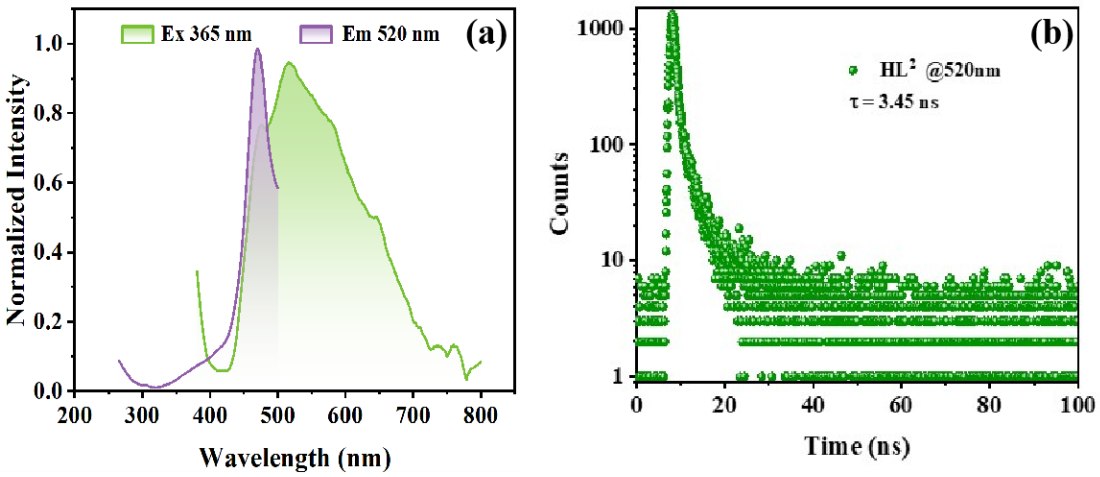


Fig. S10. (a) Fluorescence spectra of HL in the solid state. (b) The decay profile for HL in the solid state, λ_{ex} = 365 nm.

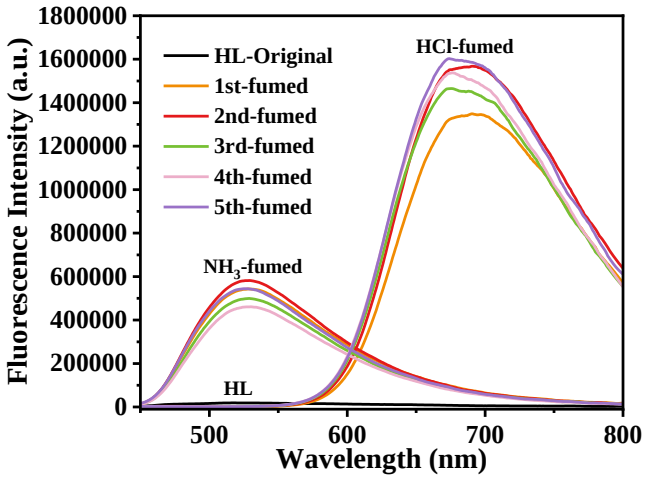


Fig. S11. Reversible acidichromism behaviors of HL with five cyclic fumigations of HCl/NH_3 vapor, λ_{ex} = 365 nm.

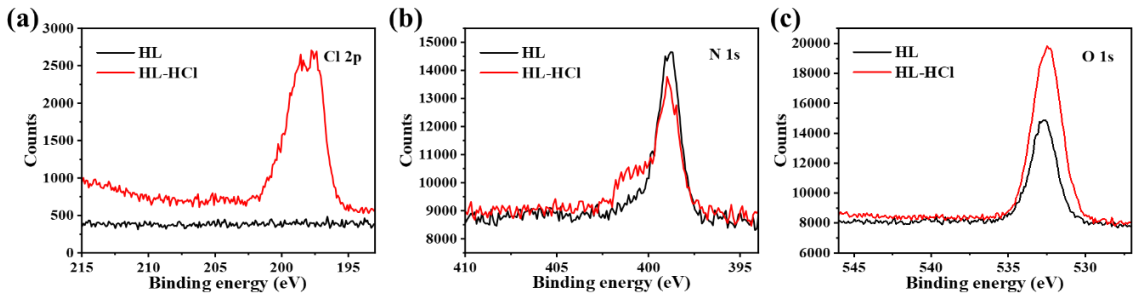


Fig. S12. XPS spectra of HL in different states.

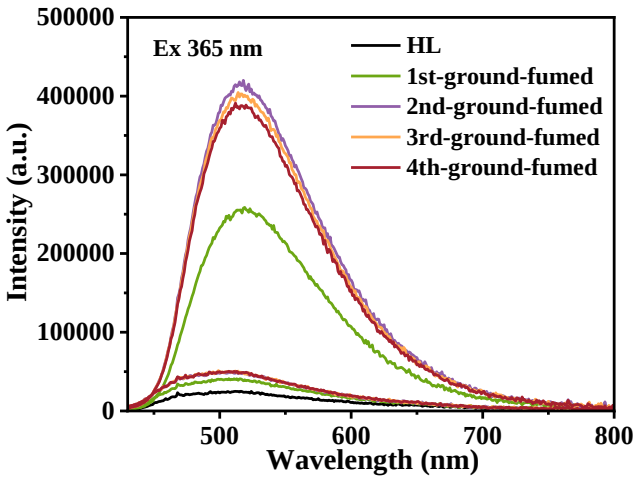


Fig. S13. Reversible mechano-responsive luminescence behavior of HL with four cycles, λ_{ex} = 365 nm.

Table S1. Crystal data and structure refinement for **HL**.

Identification code	HL
Empirical formula	$C_{42}H_{30}N_2O$
Formula weight	578.68
Temperature/K	273.15
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	9.2786(5)
b/Å	16.7335(10)
c/Å	21.5989(12)
α/°	107.902(2)
β/°	92.782(2)
γ/°	98.599(2)
Volume/Å^3	3139.3(3)
Z	4
ρ_{calc}g/cm^3	1.224
μ/mm^{-1}	0.073
F(000)	1216.0
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.01 to 45.998
Index ranges	$-7 \le h \le 10$, $-18 \le k \le 18$, $-23 \le l \le 23$
Reflections collected	20598
Independent reflections	8513 [R_{int} = 0.0561, R_{sigma} = 0.0916]
Data/restraints/parameters	8513/0/813
Goodness-of-fit on F^2	1.030

Final R indexes [I>=2σ (I)]	R_1 = 0.0620, wR_2 = 0.1426
Final R indexes [all data]	R_1 = 0.1207, wR_2 = 0.1713
Largest diff. peak/hole / e $Å^{-3}$	0.20/-0.18

Table S2. Selected bond distances (Å) and bond angles (deg) for **HL**.

HL			
O1-C8	1.353(4)	C76-C77	1.366(5)
O2-C50	1.356(4)	C52-C53	1.378(5)
N1-C9	1.357(4)	C52-C56	1.379(5)
N1-C1	1.319(4)	C62-C61	1.397(5)
N3-C51	1.368(4)	C62-C63	1.386(5)
N3-C43	1.331(4)	C49-C50	1.363(5)
N4-C55	1.321(5)	C49-C48	1.401(4)
N4-C54	1.323(5)	C5-C6	1.375(5)
C17-C18	1.389(5)	C5-C10	1.482(4)
C17-C22	1.392(5)	C31-C36	1.377(5)
C17-C16	1.464(4)	C31-C32	1.377(5)
C23-C20	1.487(4)	C53-C54	1.384(5)
C23-C24	1.491(4)	C60-C61	1.377(4)
C23-C30	1.354(4)	C60-C59	1.379(5)
C20-C21	1.386(5)	C3-C2	1.353(4)
C20-C19	1.387(5)	C79-C80	1.387(5)
C73-C72	1.492(4)	C79-C84	1.360(5)
C73-C74	1.373(5)	C67-C68	1.377(5)
C73-C78	1.386(5)	C2-C1	1.411(5)
C21-C22	1.387(4)	C14-C10	1.385(5)
C24-C25	1.382(5)	C14-C13	1.372(4)
C24-C29	1.383(5)	C15-C1	1.454(4)
C37-C30	1.498(4)	C56-C55	1.375(5)
C37-C42	1.381(5)	C63-C64	1.384(5)
C37-C38	1.369(5)	C59-C64	1.386(5)
C65-C72	1.350(5)	C59-C58	1.485(5)
C65-C66	1.501(5)	C36-C35	1.386(5)
C65-C62	1.488(4)	C45-C44	1.350(4)
C19-C18	1.380(4)	C42-C41	1.371(5)
C8-C9	1.416(5)	C43-C44	1.400(5)
C8-C7	1.357(5)	C43-C57	1.471(5)

C30-C31	1.483(5)	C26-C27	1.356(6)
C9-C4	1.421(4)	C58-C57	1.301(4)
C16-C15	1.327(4)	C78-C77	1.395(5)
C51-C46	1.418(4)	C38-C39	1.385(5)
C51-C50	1.420(5)	C10-C11	1.381(5)
N2-C13	1.317(5)	C80-C81	1.375(5)
N2-C12	1.332(5)	C71-C70	1.376(5)
C72-C79	1.489(5)	C35-C34	1.355(6)
C25-C26	1.382(5)	C34-C33	1.378(6)
C4-C5	1.425(4)	C11-C12	1.382(5)
C4-C3	1.411(5)	C32-C33	1.375(5)
C66-C67	1.380(5)	C68-C69	1.362(7)
C66-C71	1.386(5)	C41-C40	1.359(6)
C7-C6	1.387(5)	C29-C28	1.393(5)
C47-C46	1.422(4)	C27-C28	1.368(6)
C47-C52	1.487(4)	C84-C83	1.383(6)
C47-C48	1.377(5)	C39-C40	1.370(7)
C46-C45	1.406(5)	C69-C70	1.378(7)
C74-C75	1.385(5)	C81-C82	1.344(7)
C76-C75	1.358(5)	C82-C83	1.354(7)
C1-N1-C9	118.8(3)	C6-C5-C10	119.4(3)
C43-N3-C51	117.9(3)	C36-C31-C30	119.6(3)
C55-N4-C54	116.4(4)	C36-C31-C32	118.0(3)
C18-C17-C22	117.7(3)	C32-C31-C30	122.3(3)
C18-C17-C16	121.5(3)	C52-C53-C54	118.9(4)
C22-C17-C16	120.8(3)	C61-C60-C59	120.5(4)
C20-C23-C24	116.0(3)	C2-C3-C4	120.3(3)
C30-C23-C20	120.8(3)	C60-C61-C62	122.3(4)
C30-C23-C24	123.2(3)	C80-C79-C72	120.0(3)
C21-C20-C23	121.4(3)	C84-C79-C72	122.2(3)
C21-C20-C19	117.8(3)	C84-C79-C80	117.8(4)
C19-C20-C23	120.7(3)	C68-C67-C66	120.7(4)
C74-C73-C72	120.6(3)	C3-C2-C1	120.6(4)
C74-C73-C78	118.3(3)	C76-C75-C74	119.8(4)
C78-C73-C72	121.1(3)	C5-C6-C7	122.9(3)
C20-C21-C22	120.9(4)	O2-C50-C51	120.8(3)
C25-C24-C23	119.9(3)	O2-C50-C49	118.4(4)

C25-C24-C29	118.1(3)	C49-C50-C51	120.7(3)
C29-C24-C23	122.0(3)	C13-C14-C10	120.8(4)
C42-C37-C30	119.6(3)	C16-C15-C1	125.9(4)
C38-C37-C30	121.7(3)	C55-C56-C52	119.7(4)
C38-C37-C42	118.7(4)	C64-C63-C62	120.8(4)
C72-C65-C66	121.3(3)	C47-C48-C49	122.4(3)
C72-C65-C62	123.2(3)	N1-C1-C2	121.2(3)
C62-C65-C66	115.5(3)	N1-C1-C15	118.9(3)
C18-C19-C20	121.3(4)	C2-C1-C15	119.8(3)
C19-C18-C17	121.0(4)	C60-C59-C64	117.7(3)
O1-C8-C9	119.9(3)	C60-C59-C58	118.7(4)
O1-C8-C7	120.2(3)	C64-C59-C58	123.6(4)
C7-C8-C9	119.9(3)	C31-C36-C35	120.9(4)
C21-C22-C17	121.0(4)	C44-C45-C46	120.5(4)
C23-C30-C37	120.3(3)	C41-C42-C37	120.9(4)
C23-C30-C31	124.9(3)	N3-C43-C44	121.9(3)
C31-C30-C37	114.7(3)	N3-C43-C57	118.2(4)
N1-C9-C8	116.7(3)	C44-C43-C57	119.9(4)
N1-C9-C4	123.7(3)	C63-C64-C59	121.8(4)
C8-C9-C4	119.5(3)	C27-C26-C25	119.9(4)
C15-C16-C17	125.3(4)	C45-C44-C43	120.3(4)
N3-C51-C46	123.3(3)	C57-C58-C59	126.0(4)
N3-C51-C50	117.2(3)	C73-C78-C77	120.0(4)
C46-C51-C50	119.5(3)	C37-C38-C39	120.1(4)
C13-N2-C12	115.2(4)	C14-C10-C5	122.7(3)
C65-C72-C73	121.8(3)	C11-C10-C5	121.4(4)
C65-C72-C79	123.9(3)	C11-C10-C14	115.6(3)
C79-C72-C73	114.2(3)	N4-C55-C56	123.7(4)
C26-C25-C24	121.2(4)	N4-C54-C53	124.2(4)
C9-C4-C5	119.4(3)	N2-C13-C14	124.1(4)
C3-C4-C9	115.4(3)	C76-C77-C78	120.1(4)
C3-C4-C5	125.2(3)	C81-C80-C79	121.2(4)
C67-C66-C65	119.4(4)	C58-C57-C43	125.1(4)
C67-C66-C71	118.6(4)	C70-C71-C66	120.6(5)
C71-C66-C65	121.9(4)	C34-C35-C36	120.3(4)
C8-C7-C6	120.3(4)	C35-C34-C33	119.6(4)
C46-C47-C52	121.5(3)	C10-C11-C12	119.2(4)

C48-C47-C46	118.8(3)	C33-C32-C31	121.0(4)
C48-C47-C52	119.6(3)	C69-C68-C67	119.9(5)
C51-C46-C47	119.1(3)	C40-C41-C42	120.1(4)
C45-C46-C51	115.9(3)	C24-C29-C28	120.2(4)
C45-C46-C47	125.0(3)	C26-C27-C28	120.3(4)
C73-C74-C75	121.3(4)	N2-C12-C11	124.9(4)
C75-C76-C77	120.3(4)	C79-C84-C83	120.7(4)
C53-C52-C47	121.8(3)	C40-C39-C38	120.2(5)
C53-C52-C56	117.0(3)	C68-C69-C70	120.4(5)
C56-C52-C47	121.1(3)	C71-C70-C69	119.6(5)
C61-C62-C65	120.2(3)	C82-C81-C80	119.4(5)
C63-C62-C65	123.1(3)	C27-C28-C29	120.1(4)
C63-C62-C61	116.7(3)	C41-C40-C39	119.8(4)
C50-C49-C48	119.3(4)	C32-C33-C34	120.2(4)
C4-C5-C10	122.7(3)	C81-C82-C83	120.9(5)
C6-C5-C4	117.7(3)	C82-C83-C84	119.9(5)

Table S3. The optimized Cartesian Coordinates (in Å) of species studied.

Species	Cartesian coordinates			Species	Cartesian coordinates		
HL	O	-4.920453	-3.046409 -1.847008	**HL·H$^+$**	O	4.855705	-3.090031 1.653600
	H	-4.082237	-2.634245 -1.549072		H	4.016874	-2.652291 1.372736
	N	-4.101010	-0.998984 -0.437463		N	4.055482	-1.020204 0.327746
	N	-10.849471	2.135928 1.280048		N	10.872946	2.117716 -0.901158
	C	6.671718	0.798549 0.223661		C	-6.718332	0.799208 -0.207337
	C	4.509829	-0.443359 0.069806		C	-4.550538	-0.433366 -0.059002
	C	7.216636	0.239937 1.389414		C	-7.280240	0.199680 -1.344725
	H	6.557376	-0.271291 2.093647		H	-6.633078	-0.335988 -2.041817
	C	0.193415	-0.575933 -0.068027		C	-0.237662	-0.562672 0.023358
	C	5.170951	-1.758763 0.265236		C	-5.209013	-1.755797 -0.213698
	C	-8.818096	0.429295 0.318081		C	8.793543	0.383362 -0.252384
	C	2.364315	-1.478439 -0.704889		C	-2.397549	-1.471749 0.682235
	H	2.949868	-2.227293 -1.243124		H	-2.977836	-2.225085 1.219068
	C	5.217879	0.717070 -0.062286		C	-5.261900	0.728075 0.05926100
	C	0.977370	-1.516688 -0.757049		C	-1.01198200	-1.511387 0.715811
	H	0.479907	-2.293549 -1.343742		H	-0.507951	-2.294066 1.289120
	C	-5.862481	-2.259411 -1.336889		C	5.799368	-2.317743 1.175997
	C	0.865066	0.405110 0.685721		C	-0.917247	0.428943 -0.712719
	H	0.294380	1.142771 1.253552		H	-0.354558	1.171100 -1.282709
	C	-7.212315	-2.487666 -1.505339		C	7.152148	-2.593931 1.327898
	H	-7.541539	-3.349888 -2.087125		H	7.461697	-3.482987 1.878154

	C	-5.432778	-1.127835	-0.570970	C	5.382815	-1.145483	0.451115
	C	-8.782697	1.813442	0.096940	C	8.638175	1.795590	-0.208771
	H	-7.974828	2.262929	-0.484633	H	7.705616	2.240635	0.135607
	C	3.029549	-0.479911	0.021403	C	-3.072035	-0.463247	-0.025177
	C	-7.777938	-0.478922	-0.208582	C	7.737562	-0.529490	0.120704
	C	-6.385343	-0.240090	0.003081	C	6.340098	-0.256066	-0.094307
	C	9.425745	0.983205	0.754486	C	-9.478009	0.967614	-0.701407
	H	10.496680	1.051994	0.959791	H	-10.551799	1.030148	-0.892602
	C	-9.916180	-0.064313	1.034390	C	10.078487	-0.088915	-0.635402
	H	-9.997083	-1.131585	1.252383	H	10.271765	-1.158089	-0.721918
	C	8.579626	0.332130	1.652199	C	-8.646497	0.285579	-1.590008
	H	8.984631	-0.106369	2.567360	H	-9.066200	-0.182395	-2.483484
	C	-1.256515	-0.664811	-0.157436	C	1.205322	-0.655675	0.090340
	H	-1.649191	-1.485747	-0.765919	H	1.599018	-1.482216	0.690882
	C	-2.161950	0.150003	0.420555	C	2.113435	0.158125	-0.498563
	H	-1.835553	0.991855	1.037449	H	1.787198	1.004542	-1.107676
	C	2.247837	0.451971	0.727451	C	-2.298290	0.477091	-0.734024
	H	2.745194	1.222267	1.319567	H	-2.803830	1.251087	-1.313449
	C	4.706584	-2.646183	1.247510	C	-4.774933	-2.654517	-1.199309
	H	3.858262	-2.354488	1.871648	H	-3.953477	-2.367721	-1.860878
	C	-5.837156	0.799742	0.797348	C	5.788721	0.775592	-0.899800
	H	-6.501222	1.496576	1.311838	H	6.435297	1.459825	-1.451116
	C	7.529180	1.473611	-0.658230	C	-7.561118	1.504938	0.664982
	H	7.113871	1.930822	-1.559638	H	-7.133141	1.991629	1.544690
	C	4.586648	1.983747	-0.509272	C	-4.629188	2.000452	0.484271
	C	-4.476240	0.917888	0.931559	C	4.428470	0.897209	-1.030553
	H	-4.047057	1.713206	1.544487	H	4.004814	1.685261	-1.656163
	C	-3.606641	-0.003522	0.280869	C	3.546474	-0.012630	-0.373558
	C	8.894880	1.555412	-0.401051	C	-8.930497	1.578085	0.426314
	H	9.54927500	2.072884	-1.106756	H	-9.574461	2.118749	1.123859
	C	-8.146206	-1.598786	-0.939738	C	8.087720	-1.710908	0.795054
	H	-9.209720	-1.784063	-1.109667	H	9.143139	-1.922805	0.978925
	C	-9.811079	2.609644	0.595821	C	9.679534	2.628831	-0.527868
	H	-9.793806	3.692243	0.422522	H	9.604409	3.716219	-0.480162
	C	6.244843	-2.158517	-0.543392	C	-6.253537	-2.145987	0.636640
	H	6.604157	-1.483844	-1.323056	H	-6.591198	-1.460056	1.416257
	C	4.854581	3.185244	0.163996	C	-4.893792	3.190272	-0.211096
	H	5.530502	3.175309	1.022570	H	-5.570053	3.167082	-1.069059
	C	-10.891837	0.821981	1.485262	C	11.085379	0.783772	-0.955018
	H	-11.751906	0.443706	2.050441	H	12.075393	0.456321	-1.275671
	C	5.319814	-3.881296	1.438842	C	-5.388608	-3.894980	-1.350989
	H	4.952961	-4.553833	2.218033	H	-5.048281	-4.576988	-2.133838
	C	3.739630	2.017899	-1.626925	C	-3.785659	2.050843	1.603864
	H	3.540886	1.093265	-2.172630	H	-3.597425	1.136273	2.170214

	C	6.395902	-4.260712	0.637202		C	-6.434698	-4.266035	-0.506916
	H	6.874358	-5.232045	0.783320		H	-6.914822	-5.240409	-0.623196
	C	4.262014	4.377084	-0.243791		C	-4.298059	4.386795	0.176897
	H	4.471018	5.300696	0.301479		H	-4.505049	5.301939	-0.382956
	C	6.850963	-3.397270	-0.359213		C	-6.860073	-3.389683	0.491323
	H	7.684597	-3.692139	-1.001033		H	-7.671463	-3.677711	1.163757
	C	3.408323	4.394059	-1.346522		C	-3.447522	4.420341	1.282166
	H	2.947550	5.330325	-1.670376		H	-2.989215	5.362127	1.593165
	C	3.156201	3.211105	-2.041159		C	-3.200684	3.249900	1.999281
	H	2.501376	3.217982	-2.915789		H	-2.553758	3.272540	2.879505
						H	11.630196	2.750783	-1.143452

Table S4. Quantum yield of HL in different states.

	Quantum yield (%)
HL	0.1
HL-HCl	2.6
HL-HCl-NH_3	1.0

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