

Electronic Supplementary Information (ESI)

Highly sensitive and selective fluorescent sensor for copper(II) based on salicylaldehyde schiff-base derivatives with aggregation induced emission and mechanoluminescence

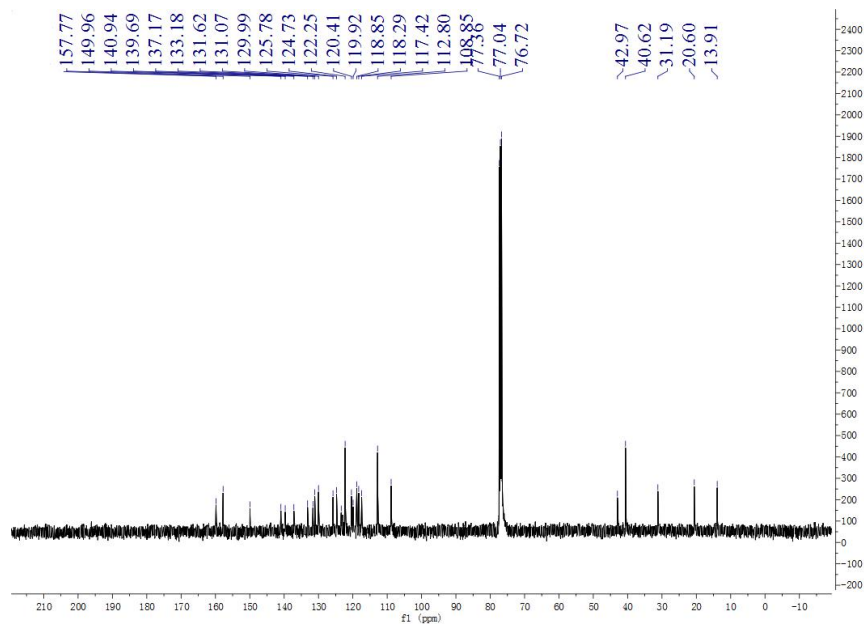
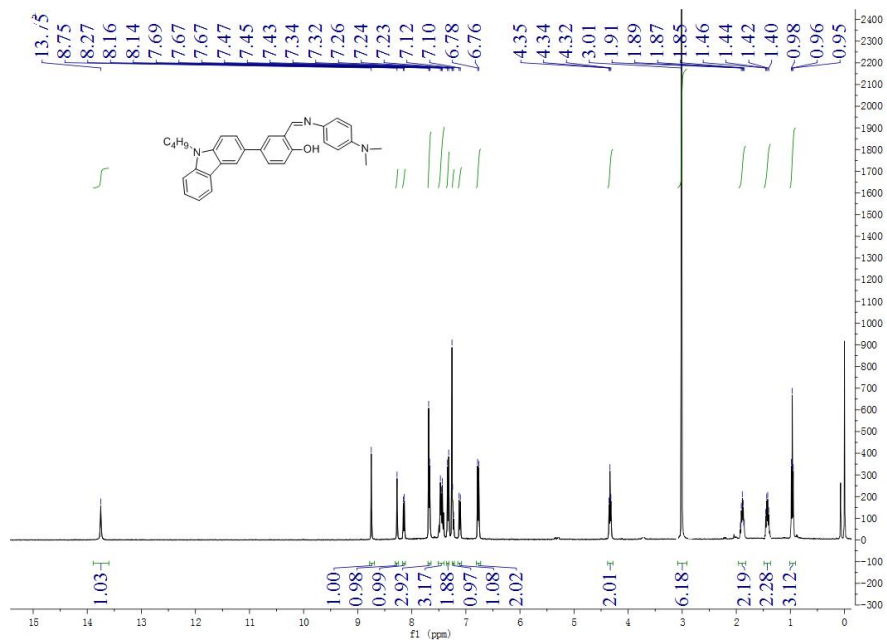
Xiaoli Yang, Wenyan Zhang, Zihan Yi, Hao Xu, Jun Wei, Lingyun Hao¹

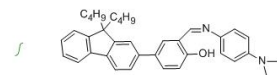
College of Material Engineering, Jinling Institute of Technology, Nanjing 211169, P. R. China

New Journal of Chemistry

*Corresponding author. Phone: +86-25-86188617. Fax: +86-25-86188617.

E-mail: haoly@jit.edu.cn





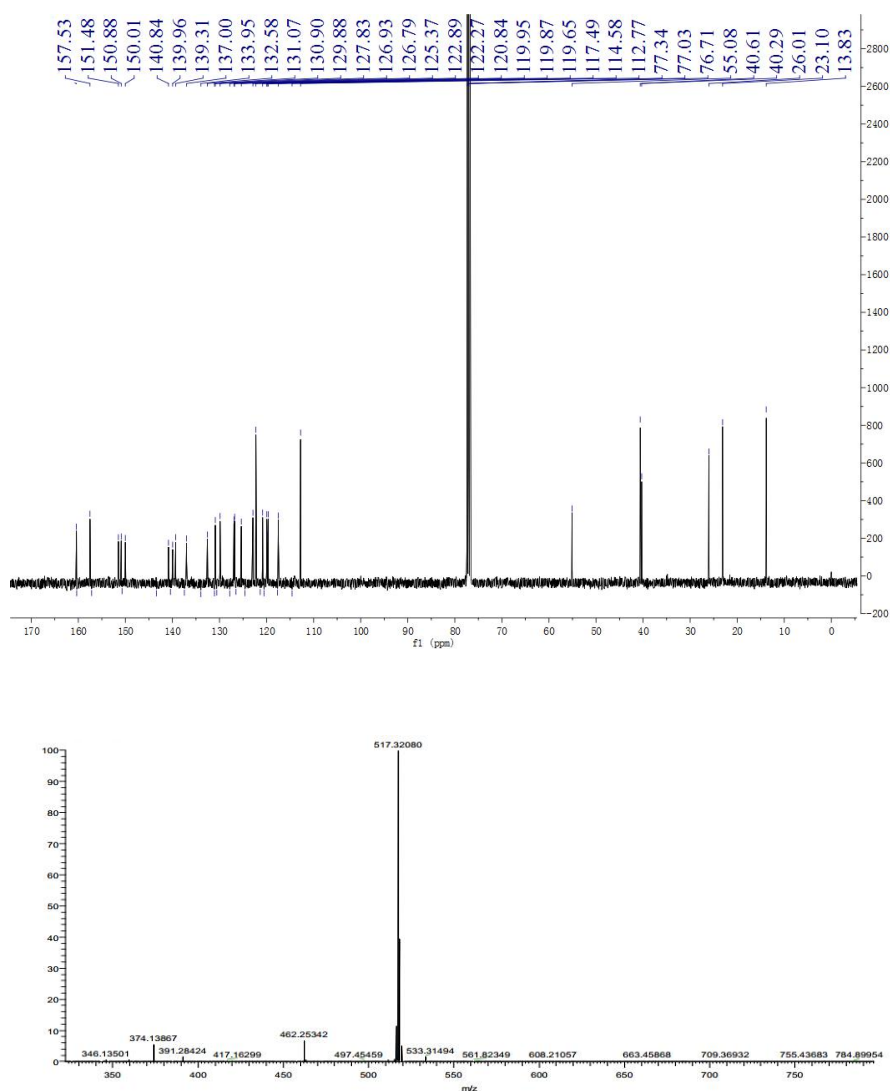


Figure S2. ^1H NMR, ^{13}C NMR and MS spectra of **A2**.

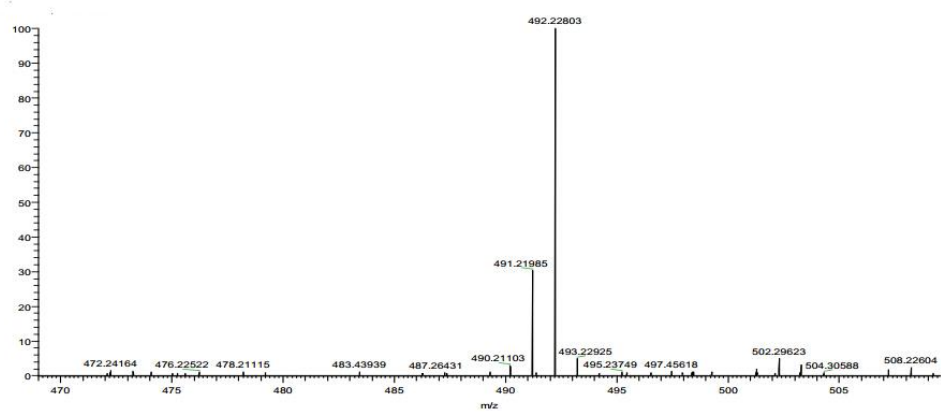
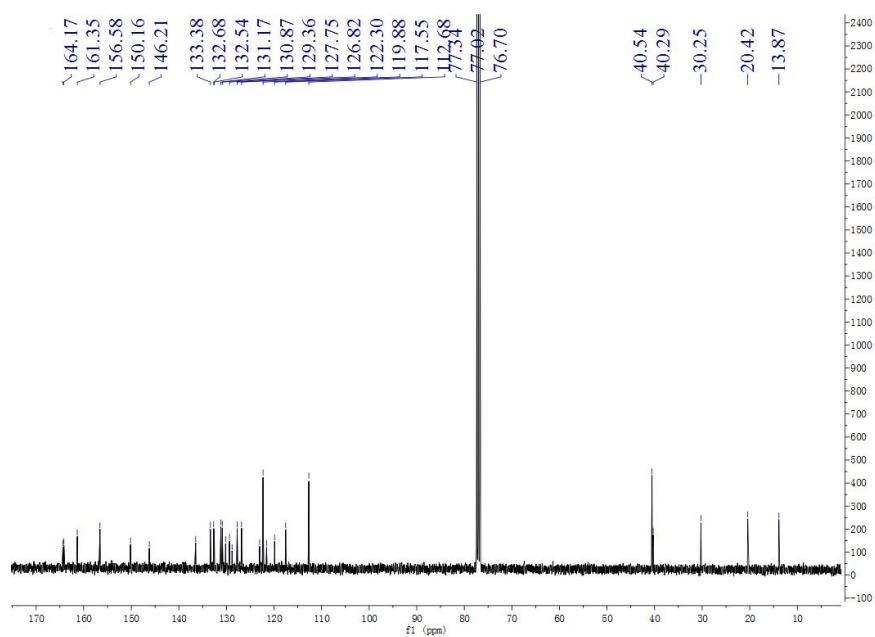
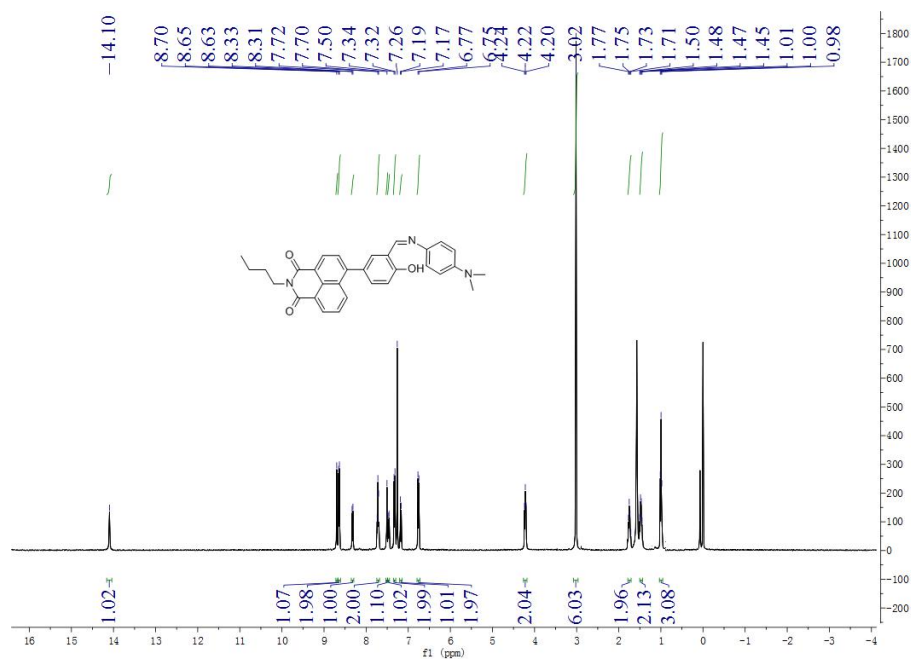


Figure S3. ¹H NMR, ¹³C NMR and MS spectra of **A3**.

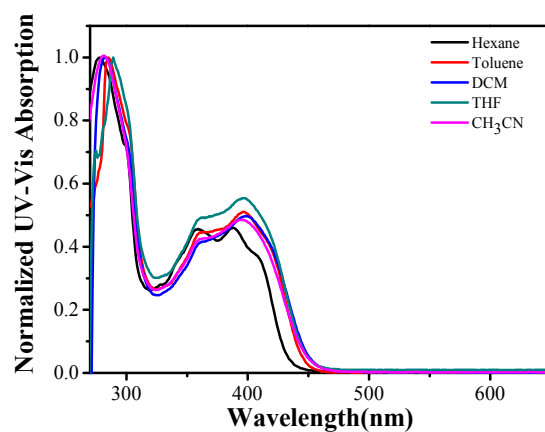


Figure S4. Normalized UV-vis absorption spectra of **A1** in different solvents.

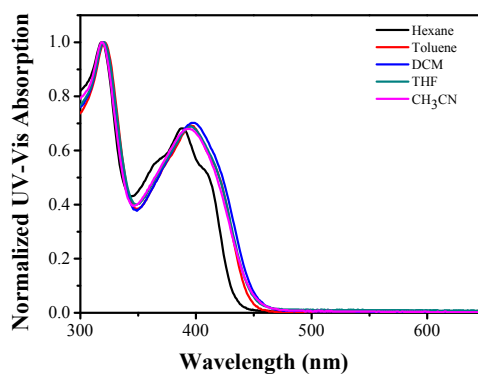


Figure S5. Normalized UV-vis absorption spectra of **A2** in different solvents.

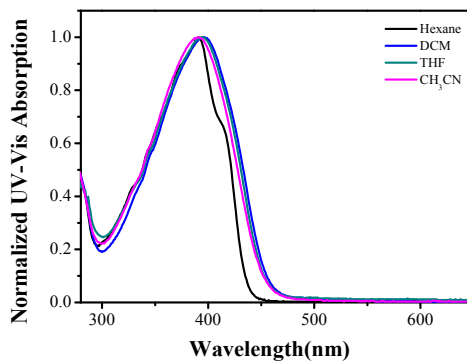


Figure S6. Normalized UV-vis absorption spectra of **A3** in different solvents.

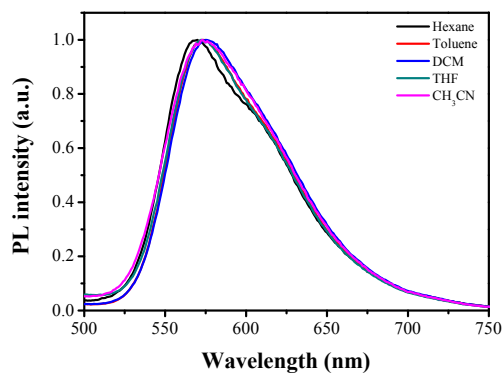


Figure S7. Normalized emission spectra of **A2** in different solvents.

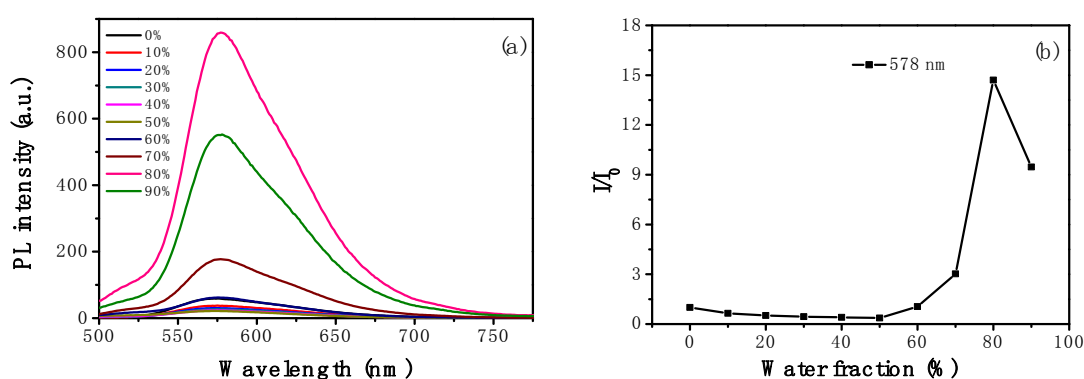


Figure S8. (a) The fluorescence spectra of **A2** in CH_3CN - H_2O with different H_2O fractions (vol., 0–90%). (b) Plot of I/I_0 vs. water content of the solvent mixture, where I_0 is the PL intensity in pure CH_3CN solution of **A2** in CH_3CN -water under irradiation of UV lamp at 365 nm.

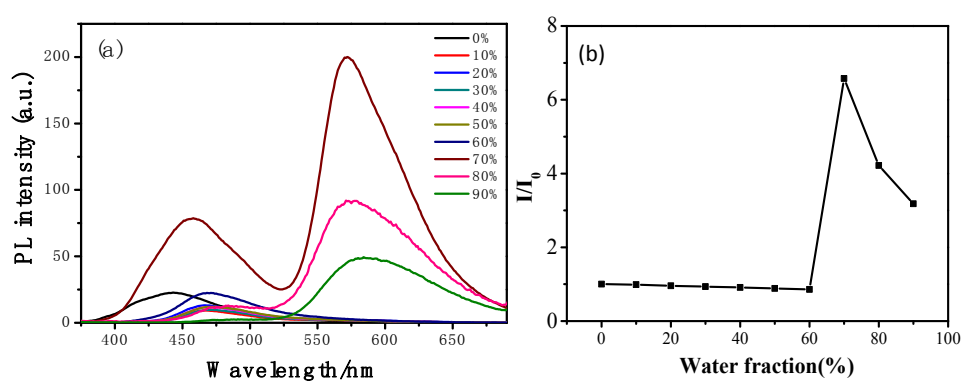


Figure S9. (a) The fluorescence spectra of **A3** in CH_3CN -water with different water fractions (vol., 0–90%). (b) Plot of I/I_0 vs. water content of the solvent mixture, where I_0 is the PL intensity in pure CH_3CN solution of **A3** in CH_3CN -water under irradiation of UV lamp at 365 nm.

Table S1. Crystallographic data of **A3** (CCDC 1557524)

A3	
formula	C ₃₁ H ₂₉ N ₃ O ₃
fw	491.57
crystal system	Triclinic
space group	P-1 (2)
<i>a</i> , Å	7.6919(13)
<i>b</i> , Å	8.8249(14)
<i>c</i> , Å	19.317(4)
<i>a</i> , deg	78.851(5)
<i>β</i> , deg	85.259(6)
<i>γ</i> , deg	82.477(5)
<i>V</i> , Å ³	1273.2(4)
<i>Z</i>	2
ρ_{caled} , g cm ⁻³	1.28215
<i>T</i> / K	296(2)
μ , mm ⁻¹	1.282
θ , deg	2.37 to 27.41
<i>F</i> (000)	520
index ranges	$-9 \leq h \leq 6$, $-10 \leq k \leq 1$, $-22 \leq l \leq 22$
data/restraints/parameters	4454/ 0 / 338
GOF (<i>F</i> ²)	0.982
<i>R</i> _{<i>I</i>} ^{<i>a</i>} , <i>wR</i> ₂ ^{<i>b</i>} (<i>I</i> > 2σ(<i>I</i>))	0.0585, 0.1296
<i>R</i> _{<i>I</i>} ^{<i>a</i>} , <i>wR</i> ₂ ^{<i>b</i>} (all data)	0.1111, 0.0537

$$R_I^a = \Sigma ||F_o| - |F_c|| / \Sigma F_o|, \quad wR_2^b = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{1/2}$$

Table S2. Summary of the molecular interactions in the crystal

Bond distances (Å)			
C(9)-N(3)	1.28(30)	C(15)-O(1)	1.35(30)
C(9)-C(10)	1.46(36)	N(3)-C(6)	1.42(34)
C(10)-C(15)	1.41(39)	C(12)-C(16)	1.49(31)
C(27)-O(3)	1.22(33)	C(3)-N(2)	1.37 (37)

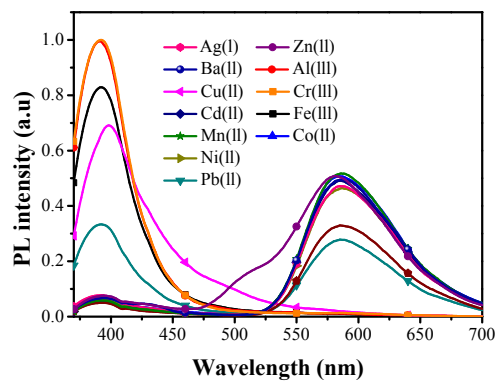


Figure S10. Fluorescence spectra of **A1** upon adding of 10 equiv. different nitrate salts in water solution (1.0×10^{-5} M, CH_3CN)

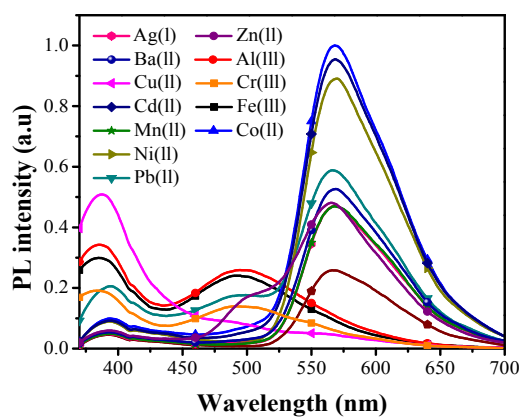
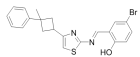
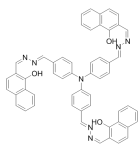
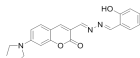
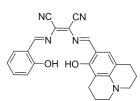
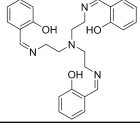
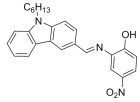
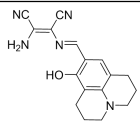
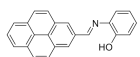
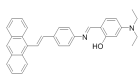
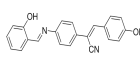
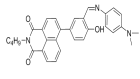


Figure S11. Fluorescence spectra of **A2** upon adding of 10 equiv. different nitrate salts in water solution (1.0×10^{-5} M, CH_3CN)

Table S3. Comparison of some Schiff base chemosensors for Cu²⁺ detection

NO	Structure of sensors	Detection limit (μM)	Linear range (μM)	Quantum yield	Interference	References
1		0.0088	0.01-570	No data	None	13
2		10.64 * 10 ⁻³	0.2-0.8	No data	None	14
3		0.27	0-10	11.5%.	None	15
4		7.3	0-80	No data	None	16
5		1.5	0-20	No data	Fe ²⁺ and Zn ²⁺	18
6		3.62	6-20	No data	Fe ³⁺	19
7		2.1	0.10-10.00	No data	None	20
8		0.97	0-50	28.4%	None	28
9		0.212	0-7.5	29.5%	None	29
10		1.5	0-10	1.5%	None	30
11		0.23	0-20	7.5%	None	This work

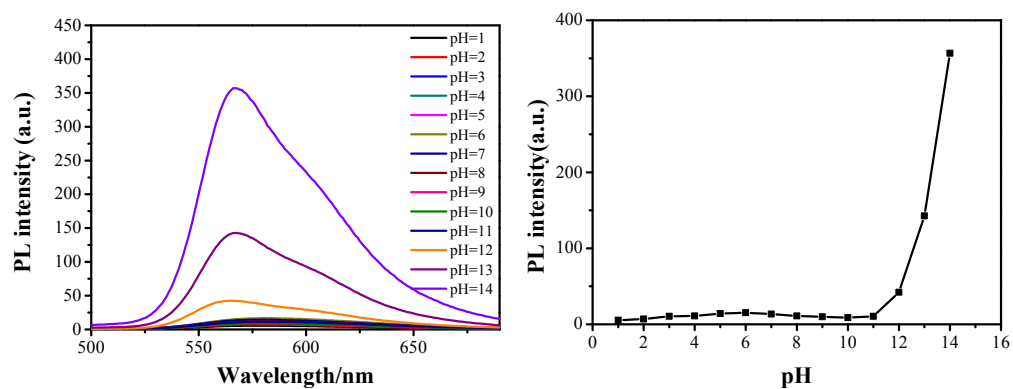


Figure S12. (a) pH-dependence of the emission spectra of **A3** in CH₃CN-buffer mixture with volume ratio 1:9; (b) change in the PL intensity with varying the pH range (1-14) at maximum PL intensity.