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Functional metallophosphors for effective charge carrier injection/transport: new robust OLED materials with emerging applications

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Table S1. A summary of the photophysical, redox, thermal and structural properties of the multifunctional metal phosphors.

	Absorption (293 K) λ_{abs} [nm] [a]	Emission λ_{em} [nm] 293 K [a]	Origin of emission	Φ_p [b]	τ_p [μs] [c]	HOMO [eV] [d]	LUMO [eV] [d]	1st $E_{1/2}^{ox}$ [V]	1st $E_{1/2}^{red}$ [V]	T_d [°C]	X-ray	Ref.
Ir-1	262 (4.76) 269 (4.72) 320 (4.56) 367 (4.60) 399 (4.58) 450 (3.87)	528	^{3}MLCT	0.13	0.10	–4.95	–1.81	0.15 0.47	–2.99	450	Yes	26
Ir-2	257 (4.57) 301 (4.53) 379 (4.50) 393 (4.51) 450 (3.82)	533	^{3}MLCT	0.14 [e]	5.00 [e]	–5.11	–1.98	0.31	–2.82 (i)	366	Yes	28
Ir-3	320 (3.35) 425 (3.02) 469 (2.86) 540 (2.21)	620	^{3}MLCT	0.28	0.81	–5.11	–2.44	0.31	–2.36	417	No	33
Ir-4	300 (3.65) 422 (3.53) 448 (3.51) 520 (2.84)	636	^{3}MLCT	0.13	1.21	–4.99	–2.34	0.19	–2.46	433	No	33
Ir-5	312 (4.14) 376 (4.18) 436 (3.73) 461 (3.75) 530 (3.04)	641	^{3}MLCT	0.12	1.40	–4.96	–2.38	0.16	–2.42	460	No	33
Ir-6	309 (4.86) 375 (4.91) 415 (4.74) 478* (3.97)	555, 595*	LC	0.12	0.08	–4.95	–2.93	0.15	–1.87	473	No	36, 37
Ir-7	297 (4.70) 387 (4.70) 408* (4.68)	564, 607*	LC	0.13	0.11	–5.06	–3.13	0.26	–1.67	432	No	38

	478* (3.84)											
Ir-8	264 (4.69) 297 (4.69) 402 (4.65) 443 (4.57)	568 603*	^{3}MLCT + LC	0.11	0.02	–5.22	–2.89	0.42	–1.91	414	No	38
Ir-9	270 (4.89) 298 (4.85) 403 (4.83) 441 (4.71)	570 605*	^{3}MLCT + LC	0.05	0.01	–5.20	–2.92	0.40	–1.88	418	Yes	38
Ir-10	321 (5.99) 336 (4.74) 405 (1.39)	548	LC	0.49	2.8	–5.02	–2.04	0.22	–2.76	441	No	39
Ir-11	266 (4.41) 284 (4.49) 330 (4.63) 396 (3.80) 446 (3.52) 475 (3.54)	556	^{3}MLCT + LC	0.19	0.55	–5.07	–2.27	0.27	–2.53 (i)	403	No	39
Ir-12	309 (5.30) 390 (4.14) 475 (3.49)	544, 583*	LC	0.26	1.3	–5.15	–2.20	0.35	–2.60 (i)	476	No	42
Ir-13	309 (5.12) 395 (3.72) 483 (3.08)	551, 589*	LC	0.21	1.1	–5.14	–2.30	0.34	–2.50 (i)	370	No	42
Ir-14	309 (5.22) 375 (4.51) 455 (4.15) 559 (3.47)	649	^{3}MLCT + LC	0.21	1.0	–5.09	–2.48	0.29	–2.32	454	No	42
Ir-15	291* (4.69) 316 (4.69) 398* (0.20)	515	^{3}MLCT	0.43	0.46	–4.95	–1.89	0.15	–2.91	477	Yes	51a
Ir-16	281 (4.74) 315 (4.88) 400* (3.20)	513	^{3}MLCT	0.43	0.18	–4.96	–1.96	0.16	–2.84	421	No	51a, 51e
Ir-17	286 (4.51) 318 (4.61) 399* (3.93)	514	^{3}MLCT	0.43	0.21	–4.93	–1.95	0.13	–2.85	473	No	51e
Ir-18	288 (4.85)	528	^{3}MLCT	0.30	0.16	–5.04	–2.08	0.24	–2.72	389	No	51e

	312 (4.87) 402* (3.80)											
Ir-19	293 (4.31) 315 (4.43) 396* (3.73)	506	^{3}MLCT	0.47	0.18	–4.88	–1.84	0.08	–2.96	479	Yes	51e
Ir-20	234 (4.95) 268 (4.73) 327 (4.66) 388 (4.44) 450* (3.69)	620	^{3}MLCT	0.19	0.68	–4.96	–2.43	0.16	–2.37	432	Yes	51d
Ir-21	234 (5.00) 267 (4.83) 328 (4.72) 393 (4.50) 455* (4.15)	624	^{3}MLCT	0.16	0.72	–4.94	–2.43	0.14	–2.37	433	No	51d
Ir-22	250 (4.57) 301 (4.62) 325 (4.66) 358 (4.40) 435 (3.34)	515	^{3}MLCT	0.41	0.42	–5.03	–1.94	0.23	–2.86	404	Yes	51e
Ir-23	300 (4.68) 325 (4.68) 356 (4.55) 434* (3.41)	514	^{3}MLCT	0.45	0.16	–5.03	–1.98	0.23	–2.82	346	No	51e
Ir-24	302 (4.30) 323 (4.34) 434* (3.64)	515	^{3}MLCT	0.41	0.27	–5.03	–1.98	0.23	–2.82	377	No	51e
Ir-25	308 (4.73) 356 (4.41) 398 (4.22) 440* (3.44)	531	^{3}MLCT	0.35	0.22	–5.10	–2.15	0.30	–2.65	374	No	51e
Ir-26	297 (4.09) 325 (4.96) 359 (4.73) 424* (3.76)	506	^{3}MLCT	0.41	0.20	–5.01	–1.92	0.21	–2.88	413	No	51e
Ir-27	239 (4.85) 322 (4.94) 375 (4.71)	567	^{3}MLCT	0.19	0.58	–5.20	–2.20	0.40	–2.60	410	Yes	51b, 51c

	405* (4.46) 475 (3.74)											
Ir-28	331 (4.82) 363 (4.69) 399 (4.50) 499* (3.11)	628	^{3}MLCT	0.30	0.79	–5.04	–2.49	0.24	–2.31	398	Yes	51d
Ir-29	265 (4.63) 321 (4.49) 364 (4.32) 405 (4.24) 500* (3.32)	628	^{3}MLCT	0.27	0.82	–5.01	–2.49	0.21	–2.31	345	No	51d
Ir-30	294 (5.17) 342 (5.26) 398 (4.73) 463 (4.18)	552 593*	LC	0.20	0.09	–5.04	–2.65	0.24		478	No	59
Ir-31	293 (4.83) 347 (5.02) 466 (3.95)	562 605*	LC	0.12	0.09	–4.96	–2.54	0.16		502	No	59
Ir-32	294 (4.64) 347 (4.69) 466 (3.60)	560 604*	LC	0.10	0.12	–5.09	–2.72	0.29		354	No	59
Ir-33	295 (5.03) 366 (5.15) 466 (4.18)	566 608*	LC	0.09	0.13	–5.06	–2.67	0.26		360	No	59
Ir-34	297 (5.01) 336 (5.16) 407 (4.09) 506 (3.96)	581	^{3}MLCT	0.25	0.12	–5.29	–2.29	0.49	–2.51		No	52
Ir-35	247 (4.66) 287 (4.71) 384 (3.95) 471 (3.22) 503 (2.83)	525	^{3}MLCT	0.70	0.18	–5.25	–2.24	0.45	–2.56	451	No	26
Ir-36	247 (4.66) 285 (4.81) 388 (4.00) 473 (3.26) 506 (2.57)	527	^{3}MLCT	0.91	0.25	–5.45	–2.48	0.65	–2.32	487	Yes	26

Ir-37	289 (4.54) 334 (4.67) 419 (3.54) 513 (3.40) 576* (2.71)	605	^{3}MLCT	0.18 [e]	2.67 [e]	–5.16	–2.39	0.36	–2.41	360	Yes	27
Ir-38	261 (4.56) 274 (4.55) 280 (4.56) 353 (3.67) 393 (3.52) 420 (3.42) 476 (3.31) 510 (2.67)	541	^{3}MLCT	0.19 [e]	2.56 [e]	–5.38	–2.40	0.58	–2.40	366	Yes	27
Ir-39	263 (4.63) 280 (4.68) 356 (3.71) 395 (3.56) 422 (3.51) 478 (3.29) 513 (2.32)	550	^{3}MLCT	0.86 [e]	2.69 [e]	–5.46	–2.54	0.66	–2.26	377	Yes	27
Ir-40	255 (4.65) 293 (4.73) 388 (4.03) 465 (3.41) 502 (2.94)	530	^{3}MLCT	0.48	0.11	–5.03	–1.92	0.23	–2.88	447	No	26
Ir-41	253 (4.69) 291 (4.76) 388 (4.07) 465 (3.40) 502 (2.75)	525	^{3}MLCT	0.53	0.11	–5.04	–1.92	0.24	–2.88	435	No	26
Ir-42	243 (4.65) 290 (4.77) 364 (4.09) 400 (3.97) 476 (2.83)	497	^{3}MLCT	0.57	0.10	–5.15	–1.97	0.35	–2.83	441	No	26
Ir-43	251 (4.76) 289 (4.67) 322 (4.63)	520	^{3}MLCT	0.42	0.15	–5.15	–2.12	0.35	–2.68	384	No	26

	376 (4.25)											
	423 (3.86)											
	499 (2.70)											
Ir-44	264 (4.60)	535	^{3}MLCT	0.39	2.44	–5.18	–2.11	0.38	–2.69	379	Yes	27
	272 (4.59)			[e]	[e]							
	281 (4.60)											
	349 (3.74)											
	414 (3.43)											
	473 (3.30)											
	508 (2.45)											
Ir-45	263 (4.69)	530	^{3}MLCT	0.40	2.17	–5.22	–2.08	0.42	–2.72	360	Yes	27
	279 (4.69)			[e]	[e]							
	347 (3.84)											
	412 (3.51)											
	467 (3.36)											
	505 (2.40)											
Ir-46	282 (4.55)	505	^{3}MLCT	0.40	1.66	–5.22	–2.00	0.42	–2.80	351	Yes	27
	403 (3.58)			[e]	[e]							
	430 (3.45)											
	481 (2.54)											
Ir-47	255 (4.53)	527	^{3}MLCT	0.52	2.53	–5.21	–2.08	0.41	–2.72	350	Yes	27
	291 (4.48)			[e]	[e]							
	322 (4.53)											
	414 (3.57)											
	445 (3.47)											
	502 (2.40)											
Ir-48	279 (4.77)	615	^{3}MLCT	0.03	0.37	–5.13	–2.82	0.33	–1.98	385	Yes	64
	301 (4.72)											
	314 (4.69)											
	364 (4.29)											
	373 (4.29)											
	475 (3.69)											
	509 (3.59)											
Pt-1	303 (4.36)	498	^{3}MLCT +	0.039	58.3	–5.12	–2.36	0.32	–2.44	305	Yes	40
	364 (4.23)	569	LC									
	382 (4.26)	628*										
	415 (4.18)											
	435 (4.21)											

Pt-2	305 (4.49) 368 (4.29) 387 (4.34) 423 (4.36) 440 (4.40)	516 570* 632*	^{3}MLCT + LC	0.086	54.6	–5.06	–2.38	0.26	–2.42	303	Yes	40
Pt-3	272 (4.26) 311 (4.36) 326 (4.43) 363* (3.92) 405 (3.82) 422 (3.80)	538 582* 624*	^{3}MLCT + LC	0.17	0.12	–5.29	–2.34	0.49 (i)	–2.46	301	Yes	40
Pt-4	309 (4.88) 364 (3.95) 406 (3.71) 422 (3.71)	540 580*	LC	0.18	8.2	–5.15	–2.38	0.35	–2.42	321	No	42
Pt-5	272 (4.44) 287 (4.53) 316 (4.42) 329 (4.44) 342 (4.50) 383 (3.76) 405 (3.71) 441 (3.08)	603	^{3}MLCT	1.0	0.88	–5.16	–2.91	0.36 (i)	–1.89	305	Yes	64
Pt-6	322 (4.51) 341 (4.46) 421* (3.48)	422* 533 573*	^{3}MLCT + LC	0.50	4.9	–5.69	–2.74	0.89		350	Yes	67
Pt-7	294 (4.90) 372 (4.88)	471 533 570*	LC	0.022	7.0	–5.42	–2.72	0.66		370	Yes	67, 68
Pt-8	293 (4.71) 370 (4.69)	429* 533 573*	LC	0.030	3.1	–5.50	–2.77	0.70		304	Yes	67
Pt-9	295 (4.72) 381 (4.65)	496* 534 571*	LC	0.017	5.4	–5.29	–2.64	0.49		341	Yes	67
Pt-10	294 (4.18) 385 (4.11)	468* 534 572*	LC	0.70	3.1	–5.05	–2.48	0.25		255	Yes	67

Pt-11	307 (4.23) 337 (4.18) 421 (4.20)	479 535	^{3}MLCT + LC	0.50	4.1	–5.09	–2.45	0.29	316	Yes	67

[a] Measured in CH_2Cl_2 at a concentration of 10^{-5} M and logε values are shown in parentheses.

[b] Relative to *fac*-[Ir(ppy)$_3$] (Φ_p = 0.40).

[c] Measured in solutions at a sample concentration of ca. 10^{-5} M.

[d] $E_{HOMO} = -(E_{ox} + 4.8)$ eV and $E_{LUMO} = -(E_{red} + 4.8)$ eV.

[e] Measured in toluene.

i = irreversible wave.

*shoulder peak.

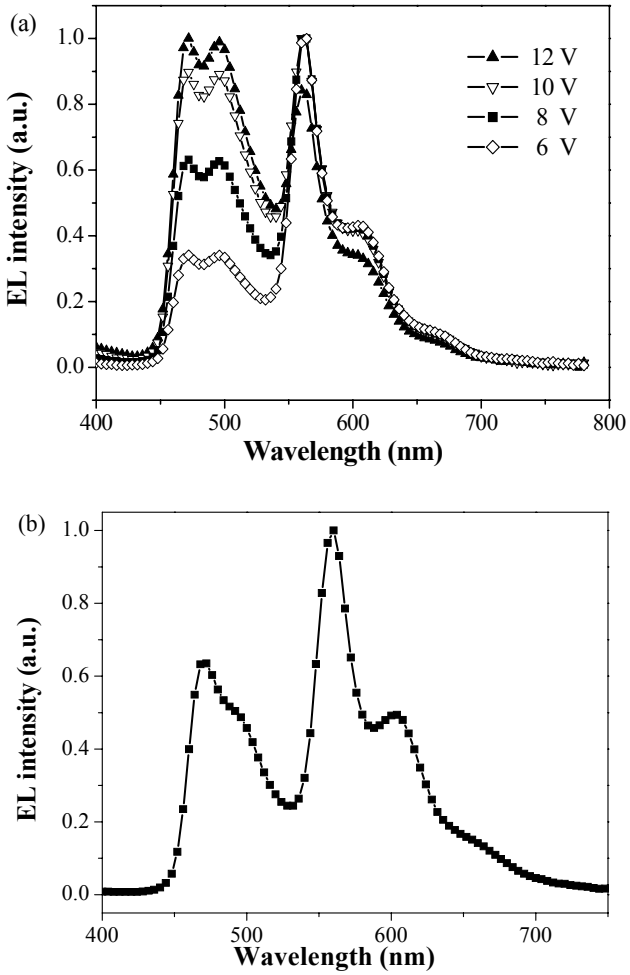

Fig. S1 Two-colour WOLEDs for (a) 5% **Ir-6** at 6–12 V and (b) 0.1% **Ir-31** at 10 V.

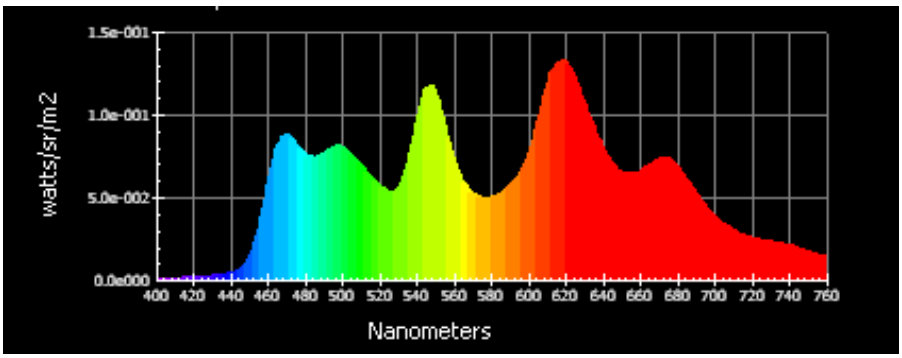

Fig. S2 EL spectra of WOLEDs with four-emissive-layer structure (blue-red-TPBI-yellow-green) with **Ir-10** as the yellow phosphor.

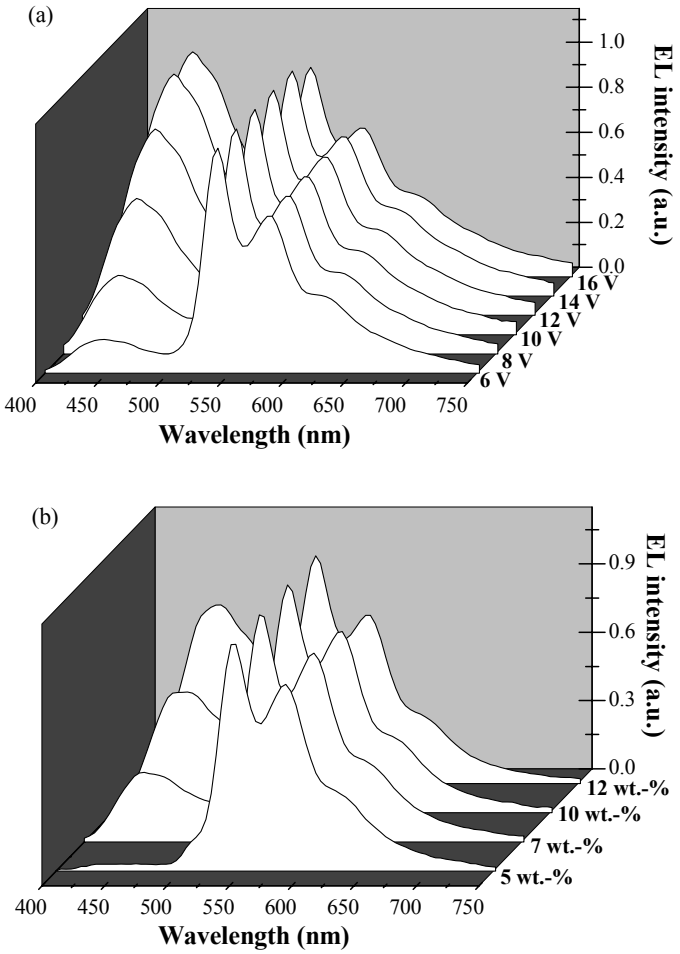

Fig. S3 (a) EL spectra of the **Pt-8**-doped device at different voltages and (b) devices with different concentrations of **Pt-9** as dopant at 8 V.