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Luminescence and Energy Transfer of a Color Tunable Phosphor: Dy^{3+}-, Tm^{3+}-, and Eu^{3+}-Coactivated $KSr_4(BO_3)_3$ for Warm White UV LEDs

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Supplementary Information

Table S1. Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters ($Å^2$) for $K(Sr, M)_4(BO_3)_3$ (*M=Dy, Tm*)

	Site	*x*	*y*	*z*	*Ueq*	Occupancy
			$K(Sr_{0.98}Dy_{0.02})_4(BO_3)_3$			
Sr1	4b	0.25	0.3555(1)	0.0624(1)	0.0113(1)	1.0000
Sr2	8c	-0.0281(1)	0.2145(1)	0.9294(1)	0.0107(1)	0.960(1)
Dy	8c	-0.0281(1)	0.2145(1)	0.9294(1)	0.0107(1)	0.040(1)
Sr3	4a	0	0	0.2829	0.0127(1)	1.0000
K	4b	0.25	0.5840(1)	0.3278(3)	0.0407(5)	1.0000
O1	4b	0.25	0.3492(1)	0.4495(3)	0.0086(5)	1.0000
O2	4b	0.25	0.5633(1)	0.9074(3)	0.0211(5)	1.0000
O3	8c	0.1371(1)	0.6720(1)	0.6699(1)	0.0041(3)	1.0000
O4	8c	0.0289(1)	0.4026(1)	0.1081(2)	0.0034(3)	1.0000
O5	8c	0.8575(1)	0.1943(1)	0.2384(2)	0.0055(3)	1.0000
O6	4a	0	0.5	0.4074(4)	0.0138(6)	1.0000
B1	4b	0.25	0.6377(3)	0.7550(6)	0.0185(10)	1.0000
B2	4b	0.25	0.3362(3)	0.6516(5)	0.0037(9)	1.0000
B3	4a	0	0.5	0.2118(6)	0.0233(10)	1.0000
			$K(Sr_{0.985}Tm_{0.015})_4(BO_3)_3$			
Sr1	4b	0.25	0.3553(1)	0.0643(1)	0.0115(1)	1.0000
Sr2	8c	-0.0284(1)	0.2148(1)	0.9312(1)	0.0098(1)	0.9732(7)
Tm	8c	-0.0284(1)	0.2148(1)	0.9312(1)	0.0098(1)	0.0267(7)
Sr3	4a	0	0	0.2829	0.0119(1)	1.0000
K	4b	0.25	0.5838(1)	0.3310(3)	0.0281(5)	1.0000
O1	4b	0.25	0.3472(1)	0.4515(3)	0.0082(5)	1.0000
O2	4b	0.25	0.5654(1)	0.9117(3)	0.0171(5)	1.0000
O3	8c	0.1364(1)	0.6727(1)	0.6688(1)	0.0068(4)	1.0000
O4	8c	0.0292(1)	0.4032(1)	0.1088(2)	0.0053(3)	1.0000
O5	8c	0.8573(1)	0.1958(1)	0.2393(2)	0.0063(4)	1.0000
O6	4a	0	0.5	0.4076(4)	0.0084(6)	1.0000
B1	4b	0.25	0.6415(3)	0.7552(6)	0.0135(9)	1.0000
B2	4b	0.25	0.3308(3)	0.6470(6)	0.0099(10)	1.0000
B3	4a	0	0.5	0.2082(6)	0.0208(10)	1.0000
			$K(Sr_{0.985}Dy_{0.01}Tm_{0.005})_4(BO_3)_3$			
Sr1	4b	0.25	0.3550(1)	0.0629(1)	0.0121(1)	1.0000
Sr2	8c	-0.0282(1)	0.2147(1)	0.9304(1)	0.0106(1)	0.976(1)
Dy1	8c	-0.0282(1)	0.2147(1)	0.9304(1)	0.0106(1)	0.014(1)
Tm	8c	-0.0282(1)	0.2147(1)	0.9304(1)	0.0106(1)	0.010(1)
Sr3	4a	0	0	0.2829	0.0116(1)	0.984(1)
Dy2	4b	0	0	0.2829	0.0116(1)	0.016(1)
K	4b	0.25	0.5834(1)	0.3262(3)	0.0332(4)	1.0000
O1	4b	0.25	0.3489(1)	0.4480(3)	0.0122(4)	1.0000
O2	8c	0.25	0.5569(1)	0.9100(3)	0.0286(4)	1.0000
O3	8c	0.1379(1)	0.6712(1)	0.6709(1)	0.0064(3)	1.0000
O4	8c	0.0277(1)	0.4040(1)	0.1093(2)	0.0058(2)	1.0000
O5	4a	0.8572(1)	0.1927(1)	0.2382(1)	0.0119(3)	1.0000
O6	4b	0	0.5	0.4025(3)	0.0047(4)	1.0000
B1	4b	0.25	0.6352(3)	0.7633(5)	0.0173(8)	1.0000
B2	4a	0.25	0.3308(2)	0.6472(4)	0.0045(7)	1.0000
B3	4b	0	0.5	0.2032(5)	0.0214(8)	1.0000

Table S2. Selected Interatomic Distances (Å) and Angles (deg) for $K(Sr, M)_4(BO_3)_3$ (M=Dy, Tm)

		$K(Sr_{0.98}Dy_{0.02})_4(BO_3)_3$			
$Sr(1)–O(1)^{i}$	2.666(2)	$Sr(3)–O(2)^{vii}$	2.9812(7)	$B(1)–O(3)^{i}$	1.433(2)
$Sr(1)–O(2)^{i}$	2.708(2)	$Sr(3)–O(3)^{v}$	2.671(1)	$B(1)–O(3)^{ii}$	1.433(2)
$Sr(1)–O(3)^{v}$	2.633(1)	$Sr(3)–O(3)^{viii}$	2.671(1)	$B(2)–O(1)^{i}$	1.399(4)
$Sr(1)–O(3)^{vi}$	2.633(1)	$Sr(3)–O(4)^{v}$	2.545(1)	$B(2)–O(5)^{vii}$	1.375(2)
$Sr(1)–O(4)^{i}$	2.5185(9)	$Sr(3)–O(4)^{viii}$	2.545(1)	$B(2)–O(5)^{viii}$	1.375(2)
$Sr(1)–O(4)^{ii}$	2.5185(9)	$Sr(3)–O(5)^{i}$	2.824(1)	$B(3)–O(4)^{i}$	1.405(2)
$Sr(1)–O(5)^{vii}$	2.595(1)	$Sr(3)–O(5)^{iv}$	2.824(1)	$B(3)–O(4)^{iv}$	1.405(2)
$Sr(1)–O(5)^{viii}$	2.595(1)	$Sr(3)–O(6)^{v}$	2.585(2)	$B(3)–O(6)^{i}$	1.346(4)
$Sr(2)(Dy)–O(1)^{vii}$	2.5636(8)	$K–O(1)^{i}$	2.935(2)	$O(2)^{i}–B(1)–O(3)^{i}$	119.79(2)
$Sr(2)\ (Dy)–O(3)^{iv}$	2.546(1)	$K–O(2)^{i}$	2.905(3)	$O(2)^{i}–B(1)–O(3)^{ii}$	119.79(2)
$Sr(2)\ (Dy)–O(3)^{v}$	2.512(1)	$K–O(3)^{i}$	2.863(2)	$O(3)^{i}–B(1)–O(3)^{ii}$	120.15(2)
$Sr(2)\ (Dy)–O(4)^{i}$	2.643(1)	$K–O(3)^{ii}$	2.863(2)	$O(1)^{i}–B(2)–O(5)^{vii}$	117.48(2)
$Sr(2)\ (Dy)–O(4)^{viii}$	2.619(1)	$K–O(5)^{iii}$	2.973(2)	$O(1)^{i}–B(2)–O(5)^{viii}$	117.48(2)
$Sr(2)\ (Dy)–O(5)^{i}$	2.484(1)	$K–O(5)^{iv}$	2.973(2)	$O(5)^{vii}–B(2)–O(5)^{viii}$	118.75(2)
$Sr(2)\ (Dy)–O(5)^{viii}$	2.539(1)	$K–O(6)^{i}$	2.9816(10)	$O(4)^{i}–B(3)–O(4)^{iv}$	118.93(2)
$Sr(2)\ (Dy)–O(6)^{v}$	2.5935(6)	$K–O(6)^{ii}$	2.9816(10)	$O(4)^{i}–B(3)–O(6)^{i}$	120.54(2)
$Sr(3)–O(2)^{v}$	2.9812(7)	$B(1)–O(2)^{i}$	1.377(4)	$O(4)^{iv}–B(3)–O(6)^{i}$	120.54(2)
		$K(Sr_{0.975}Tm_{0.015})_4(BO_3)_3$			
$Sr(1)–O(1)^{i}$	2.669(2)	$Sr(3)–O(2)^{vii}$	3.0015(8)	$B(1)–O(3)^{i}$	1.436(2)
$Sr(1)–O(2)^{i}$	2.729(1)	$Sr(3)–O(3)^{v}$	2.678(1)	$B(1)–O(3)^{ii}$	1.436(2)
$Sr(1)–O(3)^{v}$	2.624(1)	$Sr(3)–O(3)^{viii}$	2.678(1)	$B(2)–O(1)^{i}$	1.361(4)
$Sr(1)–O(3)^{vi}$	2.624(1)	$Sr(3)–O(4)^{v}$	2.548(1)	$B(2)–O(5)^{vii}$	1.382(2)
$Sr(1)–O(4)^{i}$	2.5212(9)	$Sr(3)–O(4)^{viii}$	2.548(1)	$B(2)–O(5)^{viii}$	1.382(2)
$Sr(1)–O(4)^{ii}$	2.5212(9)	$Sr(3)–O(5)^{i}$	2.842(1)	$B(3)–O(4)^{i}$	1.386(2)
$Sr(1)–O(5)^{vii}$	2.606(1)	$Sr(3)–O(5)^{iv}$	2.842(1)	$B(3)–O(4)^{iv}$	1.386(2)
$Sr(1)–O(5)^{viii}$	2.606(1)	$Sr(3)–O(6)^{v}$	2.585(2)	$B(3)–O(6)^{i}$	1.373(5)
$Sr(2)(Tm)–O(1)^{vii}$	2.5586(8)	$K–O(1)^{i}$	2.956(2)	$O(2)^{i}–B(1)–O(3)^{i}$	118.96(2)
$Sr(2)\ (Tm)–O(3)^{iv}$	2.550(1)	$K–O(2)^{i}$	2.897(3)	$O(2)^{i}–B(1)–O(3)^{ii}$	118.96(2)
$Sr(2)\ (Tm)–O(3)^{v}$	2.499(1)	$K–O(3)^{i}$	2.850(2)	$O(3)^{i}–B(1)–O(3)^{ii}$	121.43(2)
$Sr(2)\ (Tm)–O(4)^{i}$	2.646(1)	$K–O(3)^{ii}$	2.850(2)	$O(1)^{i}–B(2)–O(5)^{vii}$	119.23(3)
$Sr(2)\ (Tm)–O(4)^{viii}$	2.633(1)	$K–O(5)^{iii}$	2.964(2)	$O(1)^{i}–B(2)–O(5)^{viii}$	119.23(3)
$Sr(2)\ (Tm)–O(5)^{i}$	2.478(1)	$K–O(5)^{iv}$	2.964(2)	$O(5)^{vii}–B(2)–O(5)^{viii}$	118.06(2)
$Sr(2)\ (Tm)–O(5)^{viii}$	2.541(1)	$K–O(6)^{i}$	2.9825(9)	$O(4)^{i}–B(3)–O(4)^{iv}$	120.76(2)
$Sr(2)\ (Tm)–O(6)^{v}$	2.6003(5)	$K–O(6)^{ii}$	2.9825(9)	$O(4)^{i}–B(3)–O(6)^{i}$	119.62(3)
$Sr(3)–O(2)^{v}$	3.0015(8)	$B(1)–O(2)^{i}$	1.413(4)	$O(4)^{iv}–B(3)–O(6)^{i}$	119.62(3)
		$K(Sr_{0.985}Dy_{0.01}Tm_{0.005})_4(BO_3)_3$			
$Sr(1)–O(1)^{i}$	2.653(2)	$Sr(3)(Dy)\ –O(2)^{vii}$	2.9727(7)	$B(1)–O(3)^{i}$	1.456(2)
$Sr(1)–O(2)^{i}$	2.640(1)	$Sr(3)(Dy)–O(3)^{v}$	2.668(1)	$B(1)–O(3)^{ii}$	1.456(2)
$Sr(1)–O(3)^{v}$	2.635(1)	$Sr(3)(Dy)–O(3)^{viii}$	2.668(1)	$B(2)–O(1)^{i}$	1.389(3)
$Sr(1)–O(3)^{vi}$	2.635(1)	$Sr(3)(Dy)–O(4)^{v}$	2.544(1)	$B(2)–O(5)^{vii}$	1.368(2)
$Sr(1)–O(4)^{i}$	2.5411(8)	$Sr(3)(Dy)–O(4)^{viii}$	2.544(1)	$B(2)–O(5)^{viii}$	1.368(2)
$Sr(1)–O(4)^{ii}$	2.5411(8)	$Sr(3)(Dy)–O(5)^{i}$	2.813(1)	$B(3)–O(4)^{i}$	1.355(1)
$Sr(1)–O(5)^{vii}$	2.594(1)	$Sr(3)(Dy)–O(5)^{iv}$	2.813(1)	$B(3)–O(4)^{iv}$	1.355(1)
$Sr(1)–O(5)^{viii}$	2.594(1)	$Sr(3)(Dy)–O(6)^{v}$	2.620(2)	$B(3)–O(6)^{i}$	1.373(3)
$Sr(2)(Dy,Tm)–O(1)^{vii}$	2.5651(7)	$K–O(1)^{i}$	2.935(2)	$O(2)^{i}–B(1)–O(3)^{i}$	121.48(2)
$Sr(2)(Dy,Tm)–O(3)^{iv}$	2.555(1)	$K–O(2)^{i}$	2.884(2)	$O(2)^{i}–B(1)–O(3)^{ii}$	121.48(2)
$Sr(2)(Dy,Tm)–O(3)^{v}$	2.525(1)	$K–O(3)^{i}$	2.876(2)	$O(3)^{i}–B(1)–O(3)^{ii}$	116.21(2)
$Sr(2)(Dy,Tm)–O(4)^{i}$	2.655(1)	$K–O(3)^{ii}$	2.876(2)	$O(1)^{i}–B(2)–O(5)^{vii}$	118.97(2)
$Sr(2)(Dy,Tm)–O(4)^{viii}$	2.630(1)	$K–O(5)^{iii}$	2.995(2)	$O(1)^{i}–B(2)–O(5)^{viii}$	118.97(2)
$Sr(2)(Dy,Tm)–O(5)^{i}$	2.482(1)	$K–O(5)^{iv}$	2.995(2)	$O(5)^{vii}–B(2)–O(5)^{viii}$	119.70(1)
$Sr(2)(Dy,Tm)–O(5)^{viii}$	2.557(1)	$K–O(6)^{i}$	2.9804(7)	$O(4)^{i}–B(3)–O(4)^{iv}$	122.99(1)
$Sr(2)(Dy,Tm)–O(6)^{v}$	2.6012(4)	$K–O(6)^{ii}$	2.9804(7)	$O(4)^{i}–B(3)–O(6)^{i}$	118.50(2)
$Sr(3)(Dy)\ –O(2)^{v}$	2.9727(7)	$B(1)–O(2)^{i}$	1.379(3)	$O(4)^{iv}–B(3)–O(6)^{i}$	118.50(2)

i) x, y, z; ii) –x+1/2, y, z; iii) x+1/2,-y,z; iv) -x,-y,z; v) x,y+1/2,z+1/2; vi) -x+1/2,y+1/2,z+1/2; vii) x+1/2,-y+1/2,z+1/2; viii) -x,-y+1/2,z+1/2.

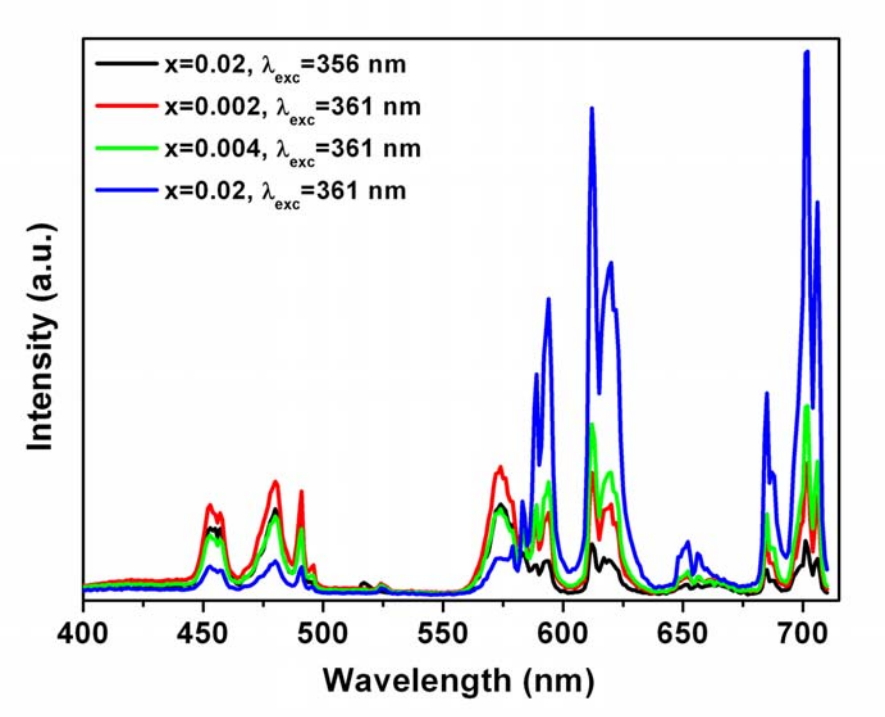

Figure S1. PL Spectra of $KSr_4(BO_3)_3$:0.01Dy^{3+}, 0.005Tm^{3+}, xEu^{3+} phosphors.

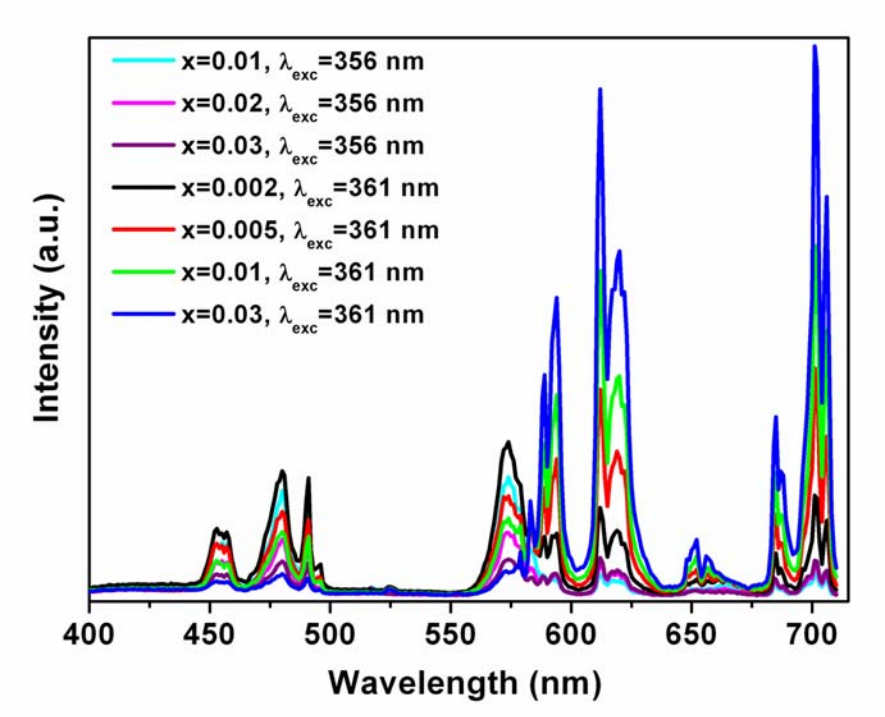

Figure S2. PL Spectra of $KSr_4(BO_3)_3$:0.015Dy^{3+}, 0.005Tm^{3+}, xEu^{3+} phosphors.

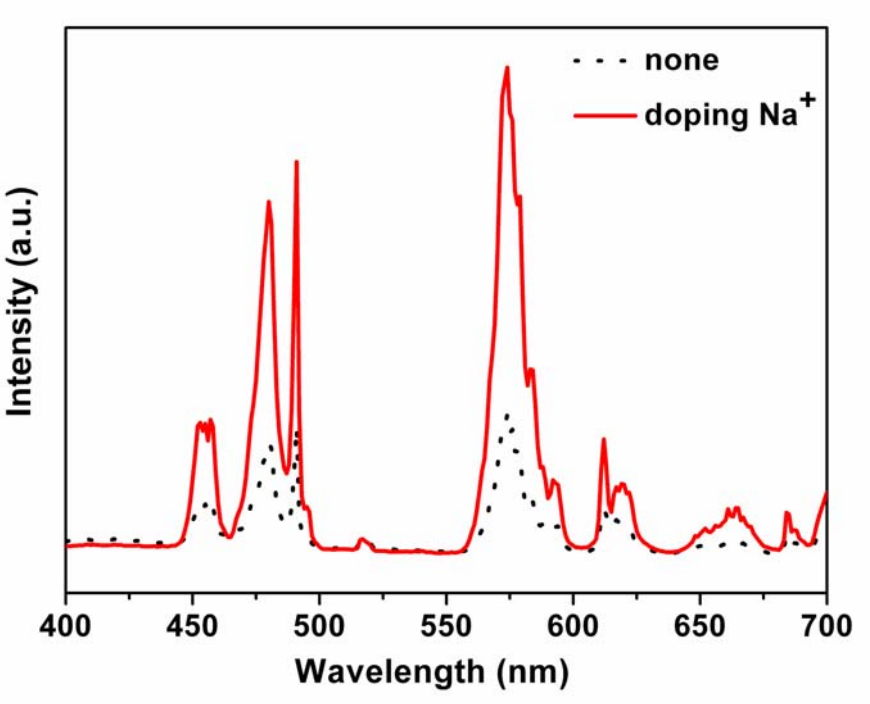

Figure S3. PL Spectra of $KSr_4(BO_3)_3$:0.015Dy^{3+}, 0.005Tm^{3+}, 0.02Eu^{3+}, 0.04Na^{+} phosphor.

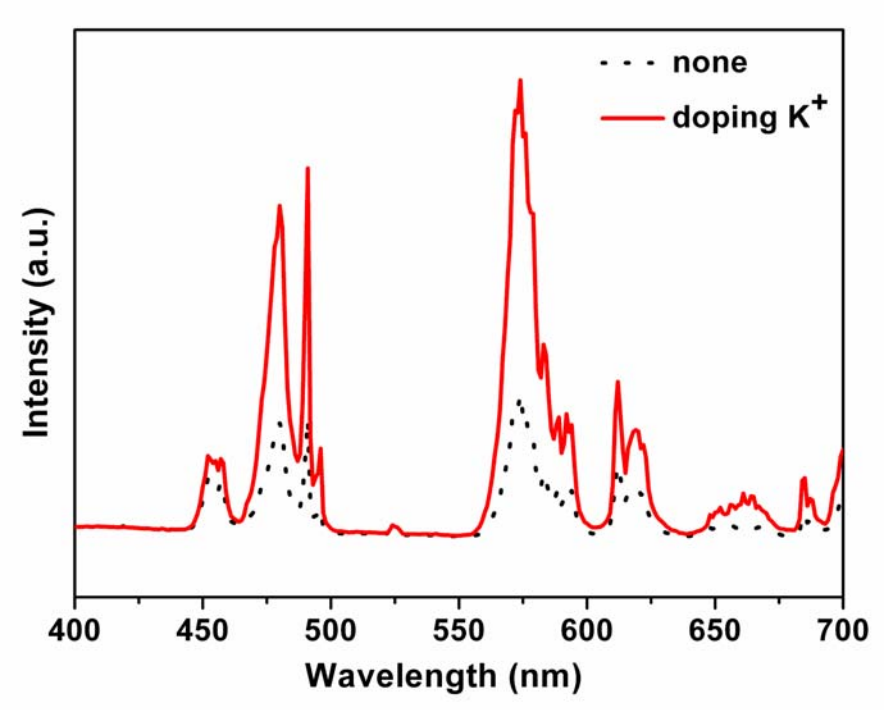

Figure S4. PL Spectra of $KSr_4(BO_3)_3$:0.015Dy^{3+}, 0.005Tm^{3+}, 0.002Eu^{3+}, 0.022K^{+} phosphor.

Figure S5. Photographs of a 368 nm UV LED chip (left) and the chip coated with $KSr_4(BO_3)_3$:0.015Dy^{3+}, 0.005Tm^{3+}, 0.02Eu^{3+} (right).

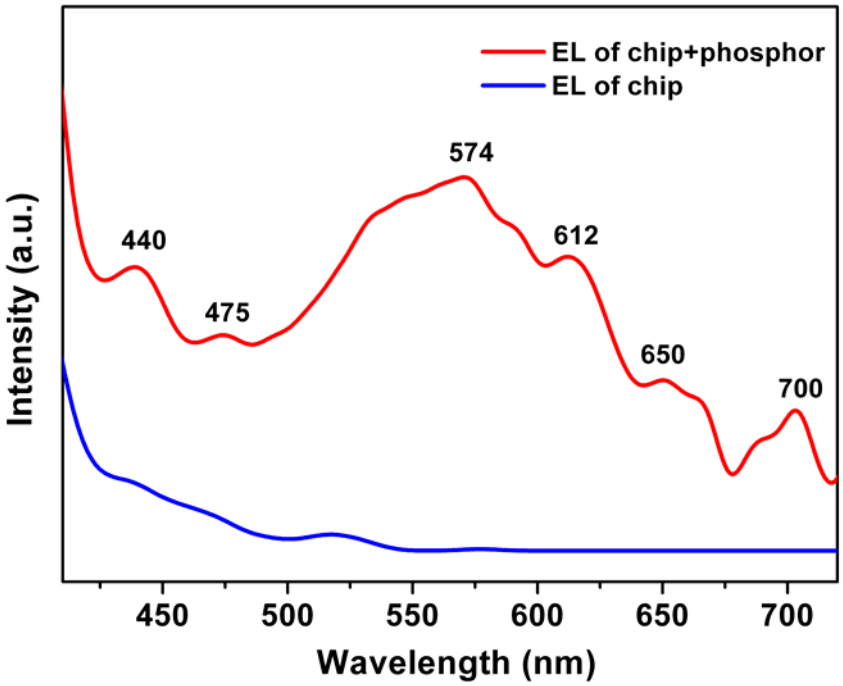

Figure S6. EL spectrum of the $KSr_4(BO_3)_3$:0.015Dy^{3+}, 0.005Tm^{3+}, 0.02Eu^{3+} phosphor coated on a 368 nm UV chip.