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Novel Narrow-Band Blue Light-Emitting Phosphor of Eu^{2+}-Activated Silicate Used for WLEDs

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Supporting Information

Experimental

Synthesis of $Rb_2HfSi_3O_9$: Eu^{2+} samples

$Rb_2HfSi_3O_9$: xEu^{2+} series phosphors were synthesized by high-temperature solid-state reaction method using Rb_2CO_3 (99.99%), HfO_2 (99.99%), SiO_2 (99.95%) and Eu_2O_3 (99.999%) as raw materials. The raw materials are accurately weighed according to the stoichiometric ratio, mixed and ground in an agate mortar for 30 minutes. After drying at room temperature, it was calcined in muffle furnace at 1150 ℃ for 4 h in air atmosphere. Finally, the sintered product was ground into fine powder for subsequent characterization.

Measurements and Characterization

The crystal structures of all samples were measured by X' Pert3 powder X-ray diffractometer (PXRD). The range of 2 θ is from 10 ° to 80 °. The general structure analysis system (GSAS) software is used to refine the XRD test data of the product by Rietveld. The morphology and energy dispersive X-ray spectroscopy (EDS) of samples, along with the elemental mappings, were collected by a scanning electron microscopy (SEM, S-340, Hitachi, Japan). The diffusion reflection spectrum (DRS) of $Rb_2HfSi_3O_9$ undoped and doped Eu^{2+} were measured using a Shimadzu UV-2700 ultraviolet spectrophotometer. The room temperature photoluminescence excitation (PLE) spectra, photoluminescence (PL) and variable temperature emission spectra of Eu^{2+}-activated $Rb_2HfSi_3O_9$ were analyzed by FS5 fluorescence spectrometer, and room temperature photoluminescence decay curves were measured by this instrument. The electron structure of the $Rb_2HfSi_3O_9$ was revealed using the density functional theory (DFT) performed

with the CASTEP code. During the DFT calculations, the Generalized Gradient Approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) was used as an exchange-correlation potential, which is based on the crystal structure of $Rb_2HfSi_3O_9$.

A prototype WLED device was fabricated by the combination of NUV-LED chip (λ_{Em} = 405 nm) and the mixture of blue-emitting $Rb_2HfSi_3O_9$: Eu^{2+}, green-emitting $(Sr, Ba)_2SiO_4$: Eu^{2+} and red-emitting $CaAlSiN_3$: Eu^{2+}. The photoluminescence properties of the WLED device were analyzed by a Hopoo HP800S photometric, colorimetric and electric test system.

Table S1 Crystal data of $Rb_2HfSi_3O_9$ from the Rietveld refinement.

Formula	$Rb_2HfSi_3O_9$
Crystal system	Hexagonal
Space group	P63/m (176)
Cell parameters	a = b = 7.0514(1) Å, c = 10.1866(4) Å
Cell volume	438.64(3) $Å^3$
Z	2

Atom	x/a	y/b	z/c	Wyck.	S.O.F.
Rb1	0.6666	0.3333	0.5655	4f	1
Hf1	0	0	0	2B	1
Si1	0.3807	0.2395	0.25	6h	1
O1	0.2766	0.231	0.1078	12i	1
O2	0.4911	0.1228	0.25	6h	1

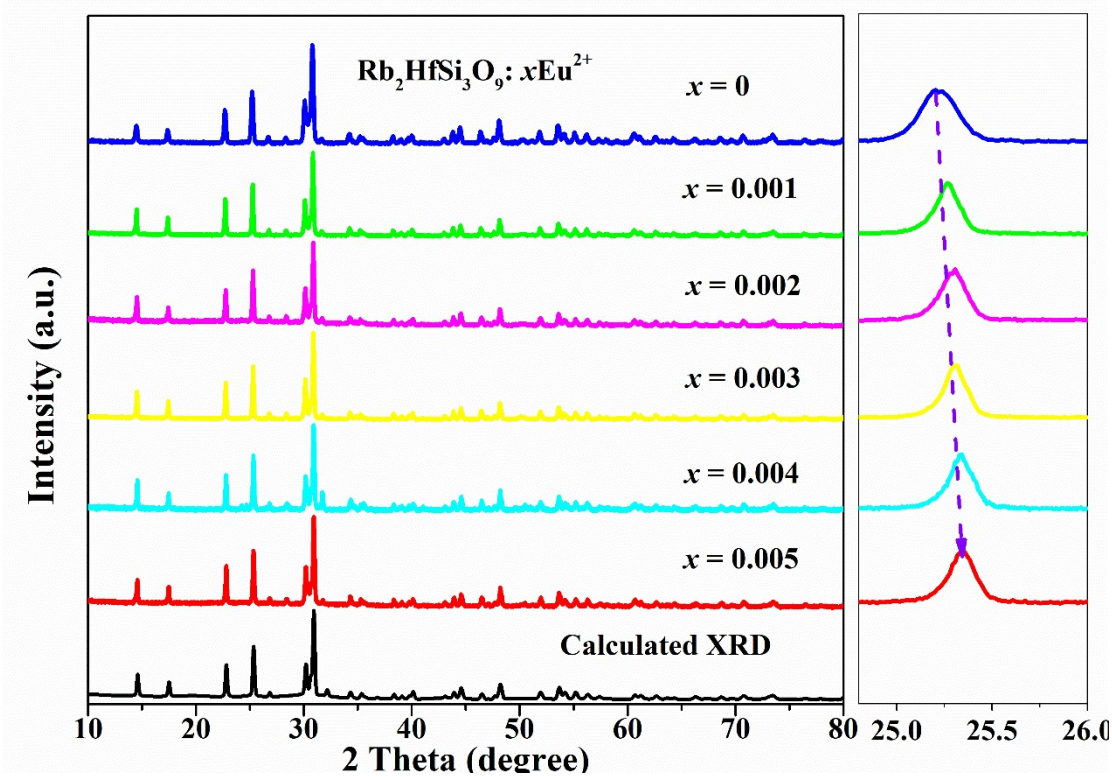

Figure S1 PXRD patterns of $Rb_2HfSi_3O_9$: xEu^{2+} ($0 \leq x \leq 0.005$) compared with calculated standard pattern of $Rb_2HfSi_3O_9$.

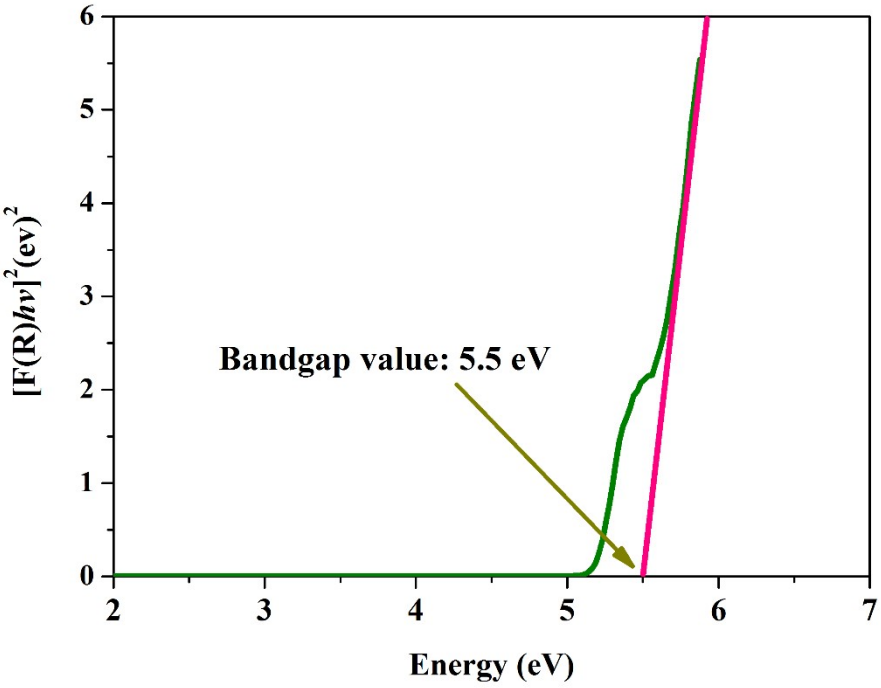

Figure S2 Relationship between $[F(R)hv]^{0.5}$ and photoenergy hv for $Rb_2HfSi_3O_9$.

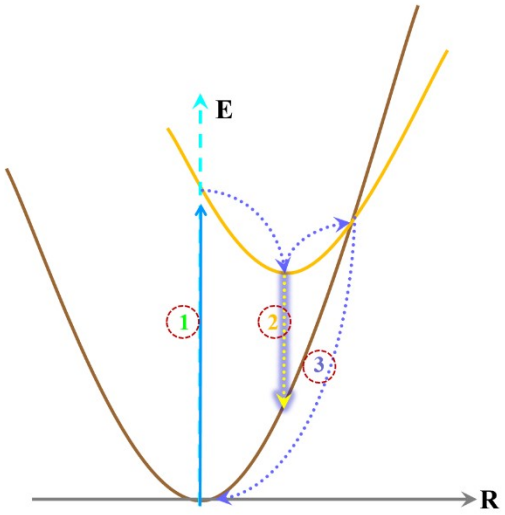

Figure S3 The configurational coordinate diagram of the ground states and the excited states of Eu^{2+}.