

Supporting Information

Doping Pb²⁺ in LaAlO₃ to generate dual emission centers and optical storage container for visible and near infrared persistent luminescence

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Table S1 Wyckoff lattice position (Wyck), atomic coordinates (x , y , z), isotropic displacement parameter (B_{iso}) and atom occupancy (Occ.) for LaAlO₃ host and LaAlO₃:0.02Pb²⁺ sample

Atom	Wyck.	x	y	z	$B_{\text{iso}} (\text{\AA}^2)$	Occ.
LaAlO ₃ host						
La	1a	0	0	0	0.018(22)	1
Al	1a	0.5	0.5	0.5	0.074(65)	1
O	3b	0.5	0.5	0	0.462(74)	1
LaAlO ₃ :0.02Pb ²⁺						
La	1a	0	0	0	0.413(36)	0.98
Al	1a	0.5	0.5	0.5	0.330(61)	1
O	3b	0.5	0.5	0	1.277(99)	1
Pb	1a	0	0	0	0.413(36)	0.02

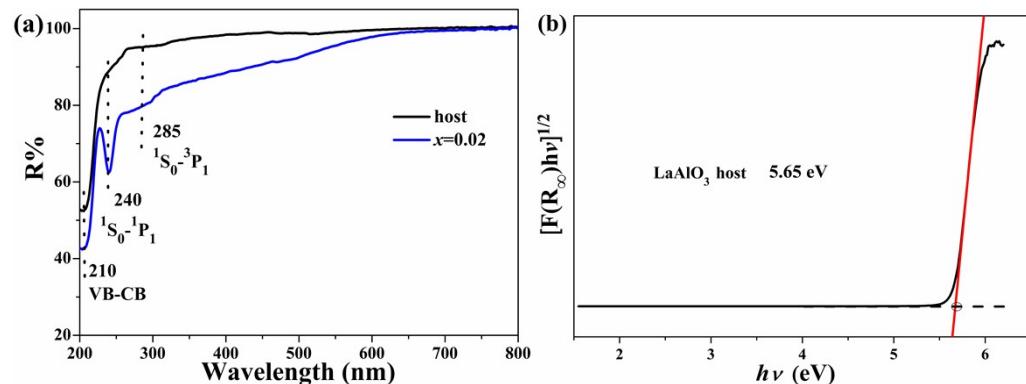


Fig. S1 (a) UV-vis diffuse reflectance apectra for LaAlO₃: x Pb²⁺ ($x=0$, 0.02) samples. (b) Extrapolation of the band gap of the LaAlO₃ host.

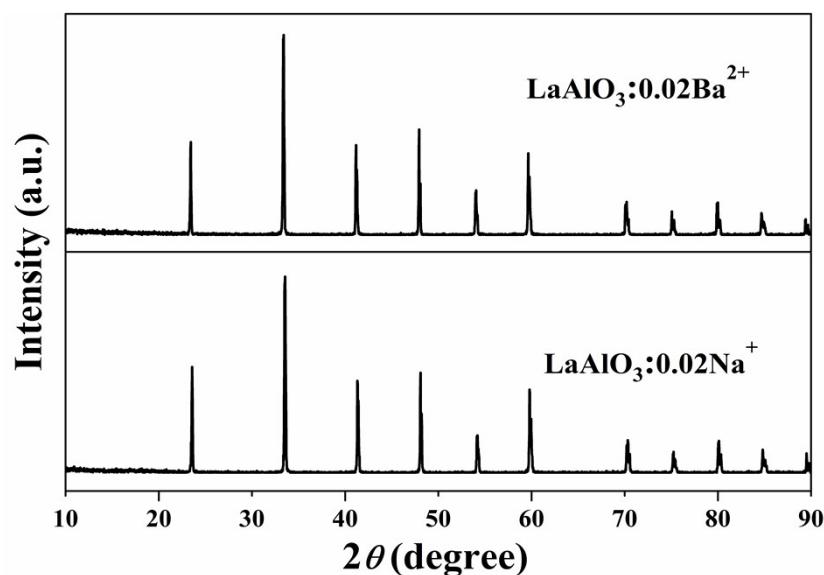


Fig. S2 XRD patterns of LaAlO₃:0.02Ba²⁺ and LaAlO₃:0.02Na⁺.

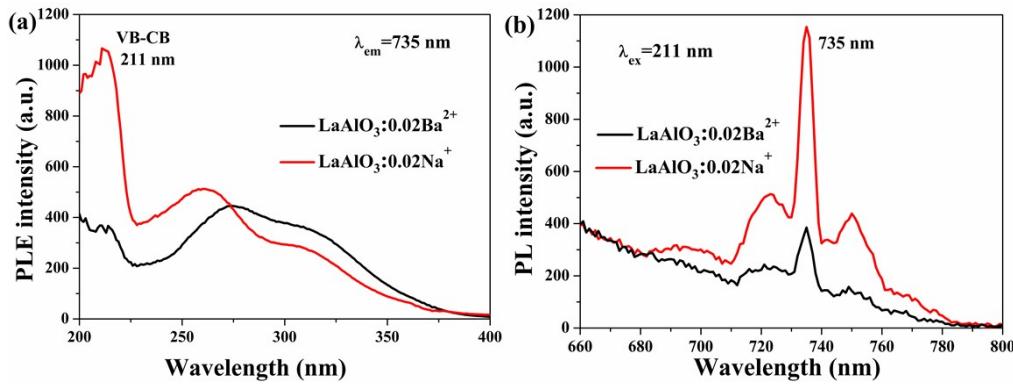


Fig. S3 PLE (a) and PL (b) spectra for $\text{LaAlO}_3:0.02\text{Ba}^{2+}$ and $\text{LaAlO}_3:0.02\text{Na}^+$ at room temperature.

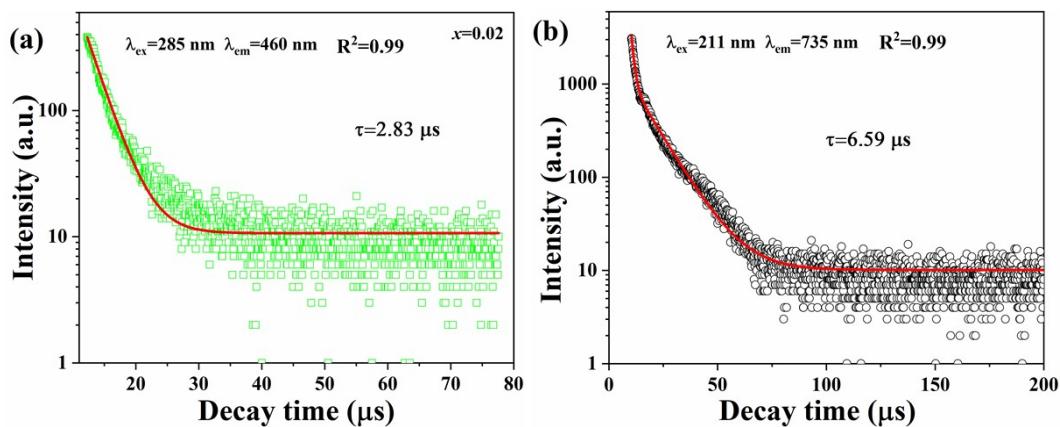


Fig. S4 PL decay curves of $\text{LaAlO}_3:0.02\text{Pb}^{2+}$.

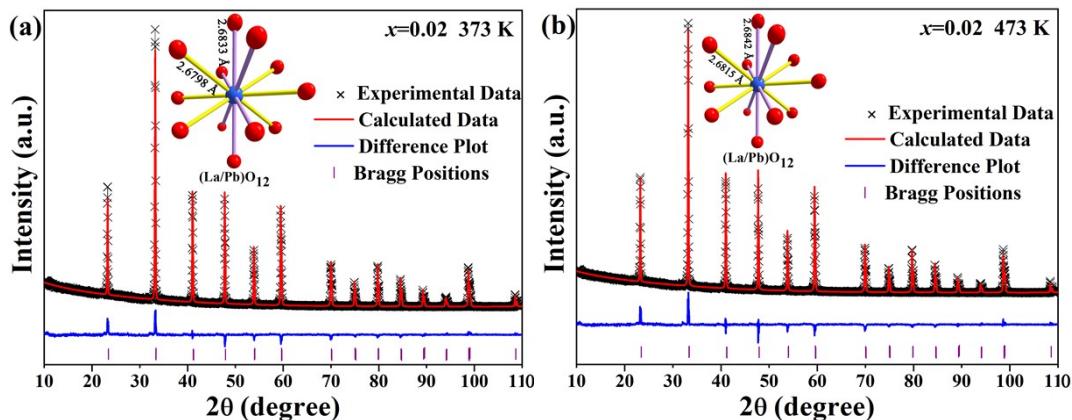


Fig. S5 Rietveld refinement of high temperature XRD patterns of $\text{LaAlO}_3:0.02\text{Pb}^{2+}$ sample at 373 K (a) and 473 K (b).

Table S2 Main parameters for Refinement of LaAlO₃:0.02Pb²⁺ sample at 298 K, 373 K and 473 K

Temperature (K)	<i>a</i> (Å)	β (°)	<i>V</i> (Å ³)	<i>R</i> _{exp}	<i>R</i> _{wp}	<i>R</i> _p	χ^2
298	3.7913(1)	90.086(1)	54.497(1)	6.90%	8.72%	5.08%	1.26
373	3.7923(1)	90.074(1)	54.541(1)	3.6%	7.34%	5.55%	2.04
473	3.7942(3)	90.057(6)	54.619(2)	3.62%	7.20%	5.41%	1.99