

Lead-Free $\text{Rb}_2\text{SnCl}_6\text{:Bi}$ Perovskite Nanocrystals for Luminescence Emission

Sarmad Ahmad Qamar[†], Tsai-Wei Lin[†], Yi-Ting Tsai[†], and Chun Che Lin^{†,‡,}*

[†] Institute of Organic and Polymeric Materials, National Taipei University of Technology, Taipei 106344, Taiwan.

[‡] Research and Development Center for Smart Textile Technology, National Taipei University of Technology, Taipei 106344, Taiwan.

**Author to whom correspondence should be addressed. E-mail: cclin0530@mail.ntut.edu.tw*

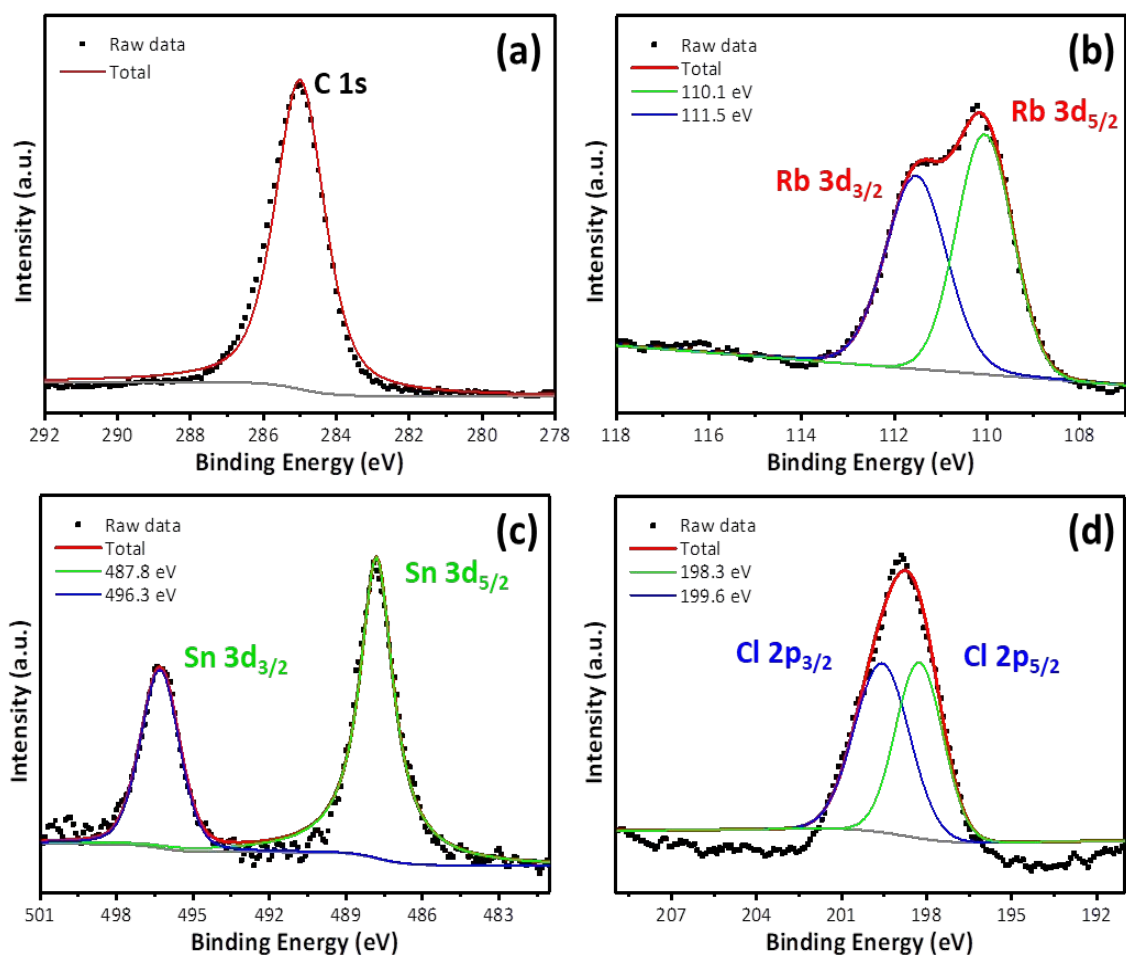


Figure S1. High-resolution XPS spectra of pure Rb_2SnCl_6 for (a) C 1s; (b) Rb 3d; (c) Sn 3d; and (d) Cl 2p high-energy discrimination spectra.

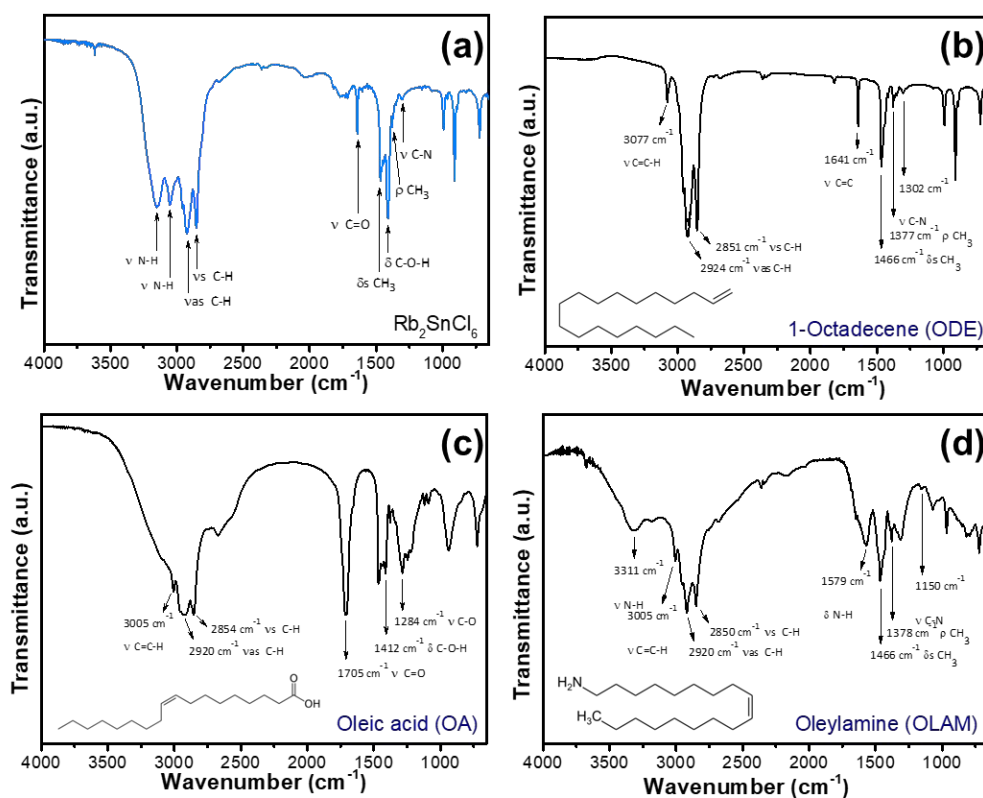


Figure S2. FT-IR spectra of (a) Rb_2SnCl_6 perovskites; (b, c, and d) reference spectra of 1-octadecane (ODE), oleic acid (OA), and oleylamine (OLAM) for comparison.

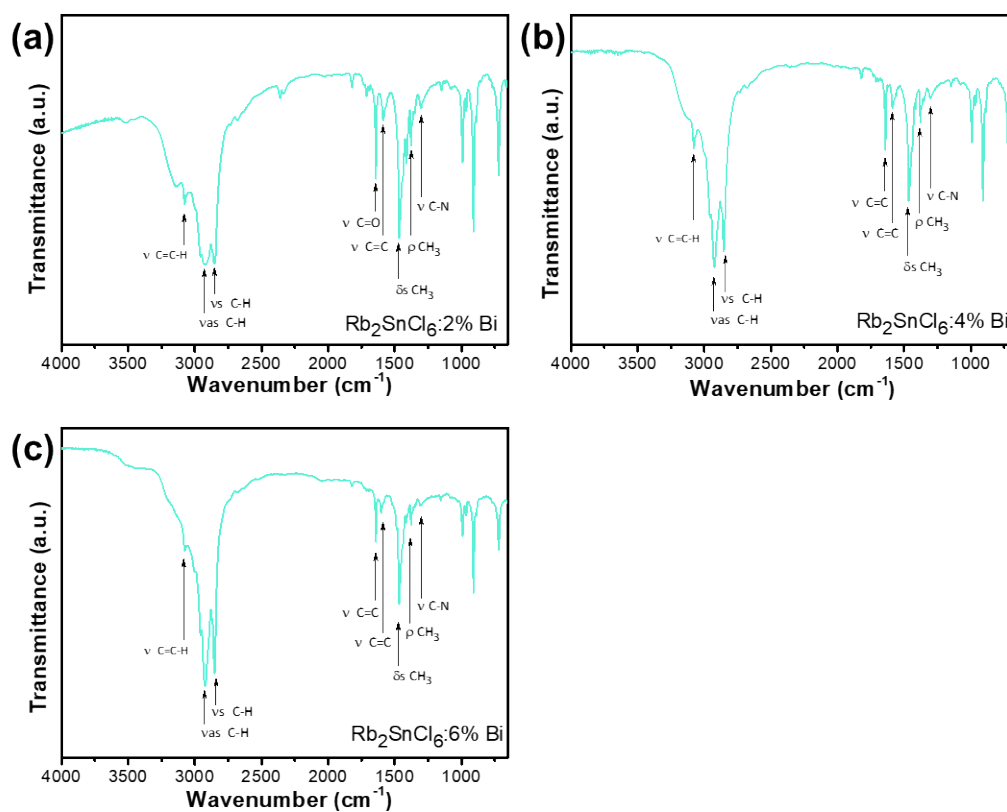


Figure S3. FT-IR spectra of newly developed perovskite nanocrystals $\text{Rb}_2\text{SnCl}_6:\text{X}\%\text{Bi}$ of (a) $\text{X} = 2$; (b) $\text{X} = 4$; and (c) $\text{X} = 6$.

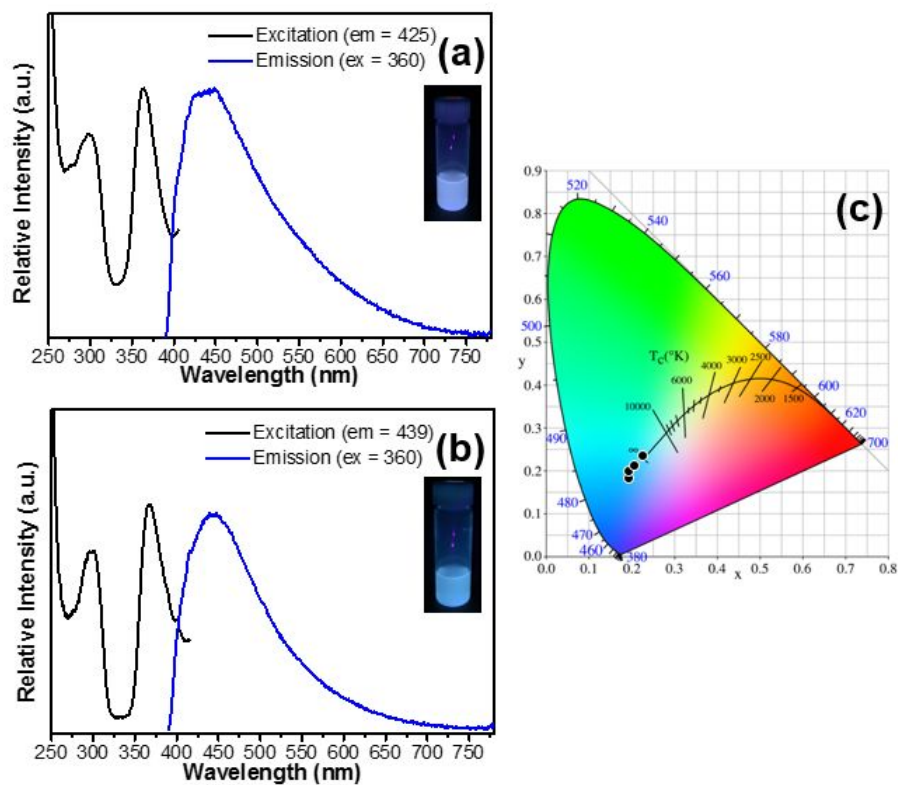


Figure S4. Excitation and emission spectra of (a) Rb_2SnCl_6 :2%Bi; (b) Rb_2SnCl_6 :6%Bi, & (c) location of Rb_2SnCl_6 :X%Bi in CIE 1931 chromaticity diagram.

Table S1. Structural parameters of Rb₂SnCl₆ nanocrystals determined by Rietveld refinement of the corresponding XRD pattern.

Cell Parameters						
Space group: <i>Fm-3m</i> (225)			Reliability values			
a (Å)	10.1218 (3)		R_{wp} (%)		8.64	
V (Å ³)	1037.00 (2)		R_p (%)		5.61	
Z	4		R_{exp} (%)		4.09	
Rb-Cl	3.580 (1)		χ^2		2.11	
Sn-Cl	2.443 (2)		R (F ²) (%)		7.05	
Fractional atomic coordinates						
Atoms	x	y	z	Occ	U_{iso}	Site
Rb	0.25000	0.25000	0.25000	1.000	0.088	8
Sn	0.00000	0.00000	0.00000	1.000	0.070	4
Cl	0.24133	0.00000	0.00000	1.000	0.081	24

Table S2. Binding energy of Rb, Sn, Cl, and Bi among Rb₂SnCl₆ and Rb₂SnCl₆:4%Bi nanocrystals.

Cpd.	Binding Energy (eV)							
	Rb		Sn		Cl		Bi	
	$3d_{5/2}$	$3d_{3/2}$	$3d_{5/2}$	$3d_{3/2}$	$2p_{5/2}$	$2p_{3/2}$	$4f_{7/2}$	$4f_{5/2}$
Rb ₂ SnCl ₆	110.1	111.5	487.8	496.3	198.3	199.6	-	-
Rb ₂ SnCl ₆ :4%Bi	109.7	111.1	487.1	495.6	198.4	199.8	159.6	164.8

Table S3. Position of Rb₂SnCl₆:X%Bi (X = 0, 2, 4, and 6) in CIE 1931 chromaticity diagram.

Nanocrystals	X-axis on CIE diagram	Y-axis on CIE diagram
Rb ₂ SnCl ₆	0.1924	0.1911
Rb ₂ SnCl ₆ :2%Bi	0.1934	0.1941
Rb ₂ SnCl ₆ :4%Bi	0.2235	0.2360
Rb ₂ SnCl ₆ :6%Bi	0.2038	0.2101

Table S4. Fluorescence decay analysis of Rb_2SnCl_6 perovskites nanocrystals.

Parameter	Value	Conf. Lower	Conf. Upper
A_1 (Cnts)	3950.51	-74.1987	+74.1987
τ_1 (ns)	0.73334	-0.01166	+0.01166
A_2 (Cnts)	4454.36	-47.9737	+47.9737
τ_2 (ns)	2.73395	-0.06077	+0.06077
A_3 (Cnts)	1537.33	-60.7045	+60.7045
τ_3 (ns)	9.02262	-0.21564	+0.21564

Table S5. Fluorescence decay analysis of $\text{Rb}_2\text{SnCl}_6\text{:4\%Bi}$ perovskites nanocrystals.

Parameter	Value	Conf. Lower	Conf. Upper
A_1 (Cnts)	5745.19	-32.4380	+32.4380
τ_1 (ns)	0.93414	-0.01059	+0.01059
A_2 (Cnts)	446.412	-32.6435	+32.6435
τ_2 (ns)	10.6624	-1.61286	+1.61286