

Supporting information

Tunable cathodoluminescence over entire visible window from all-inorganic perovskite CsPbX₃ 1D architecture

T. Paul¹, B.K. Chatterjee¹, S.Maiti^{2†}, S.Sarkar³, N. Besra³, B.K. Das³, K.J.Panigrahi¹, S. Thakur¹,
U.K.Ghorai⁴ and K.K. Chattopadhyay^{1, 4, *}

¹ *School of Materials Science and Nanotechnology, Jadavpur University, Kolkata 700032, India.*

² *St. Thomas College of Engineering & Technology Kolkata 700032, India.*

³ *Departments of Physics, Jadavpur University, Kolkata 700032, India.*

⁴ *Department of Industrial Chemistry and Applied Chemistry, Swami Vivekananda Research Center, Ramakrishna Mission Vidyamandira, Belurmath, Howrah- 711202, India*

[†] *Present address: CENIMAT/I3N, Faculdade de Ciências e Tecnologia, FCT Portugal*

*Corresponding author Tel.: +91 33 2413 8917. Fax: +91 33 2414 6007. E-mail: kalyan_chattopadhyay@yahoo.com.

Characterization:

Powder x-ray diffraction (XRD) patterns of the synthesized samples are recorded on a Bruker D8 diffractometer with Cu-K_α radiation of wavelength 1.5404 Å at room temperature. Field emission scanning electron microscope (FESEM) images are taken to determine the size and morphology of the as-synthesized samples by a HITACHI S4800 electron microscope and energy dispersive x-ray spectroscopy (EDX) is used for elemental study by the same. Precise dimension, morphology of the nanostructures and the lattice images are acquired by high resolution transmission electron microscopy (HRTEM, JEOL JEM 2010). UV-Vis reflectance spectra of the samples are recorded by using a Jasco V670 spectrophotometer. Photoluminescence spectra of the samples are recorded on a Horiba Jobin Yvon Fluorolog-3 spectrophotometer and Edinburgh F980 instrument. Room temperature cathodoluminescence spectra are recorded with

Gatan Mono CL3 equipment attached to the FESEM using a beam accelerating voltage ranging from 1 kV to 15 kV.

Computational details:

The Density Functional calculations were carried out using Vienna *Ab initio* Simulation Package (VASP) [1-4] with projector-augmented-wave (PAW) [5] approach. Perdew Burke Ernzerhof (PBE) functional [6] is implemented to describe the exchange-correlation energy functional within the generalized gradient approximation with Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional [7]. Plane wave basis set up to energy cut off 262 eV is used during calculation. For the geometry optimization brillouin zone integrations were performed with k point spacing of $0.13/\text{\AA}$ centered at the Γ point. During geometry optimization both cell dimensions and atom positions were allowed to relax until the total energy converged to less than 10^{-4} eV/ atom. **Fig. 1:**

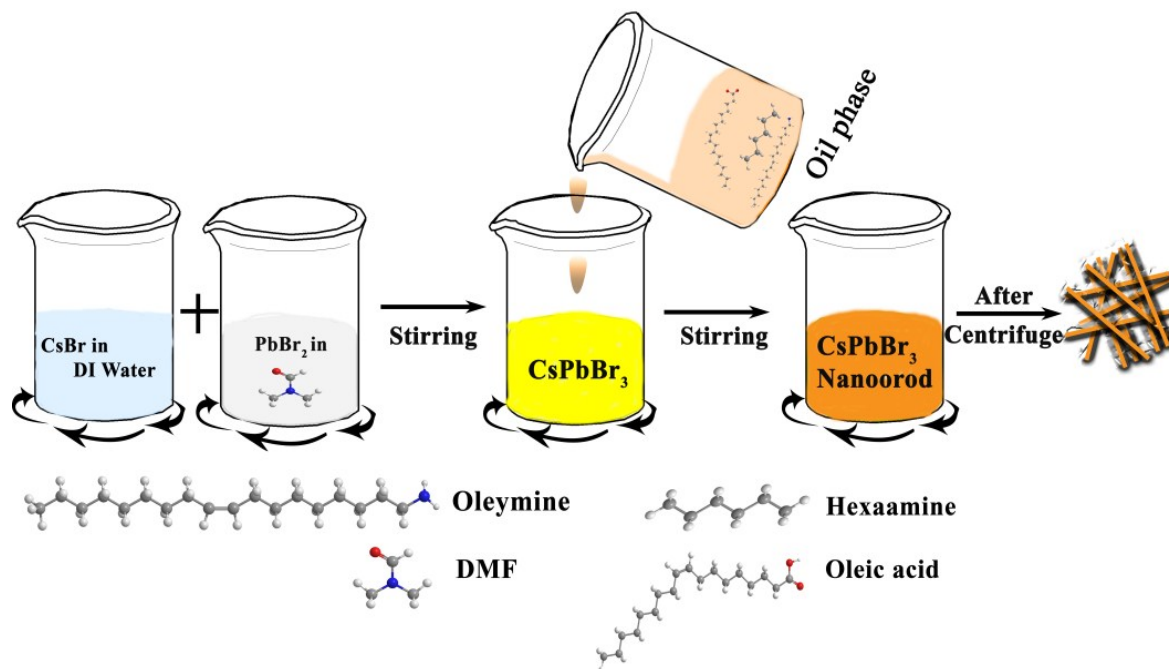


Figure S1: Schematic illustration of room temperature synthesis of all-inorganic perovskite CsPbX₃ (X =Cl, Br, I) rods.

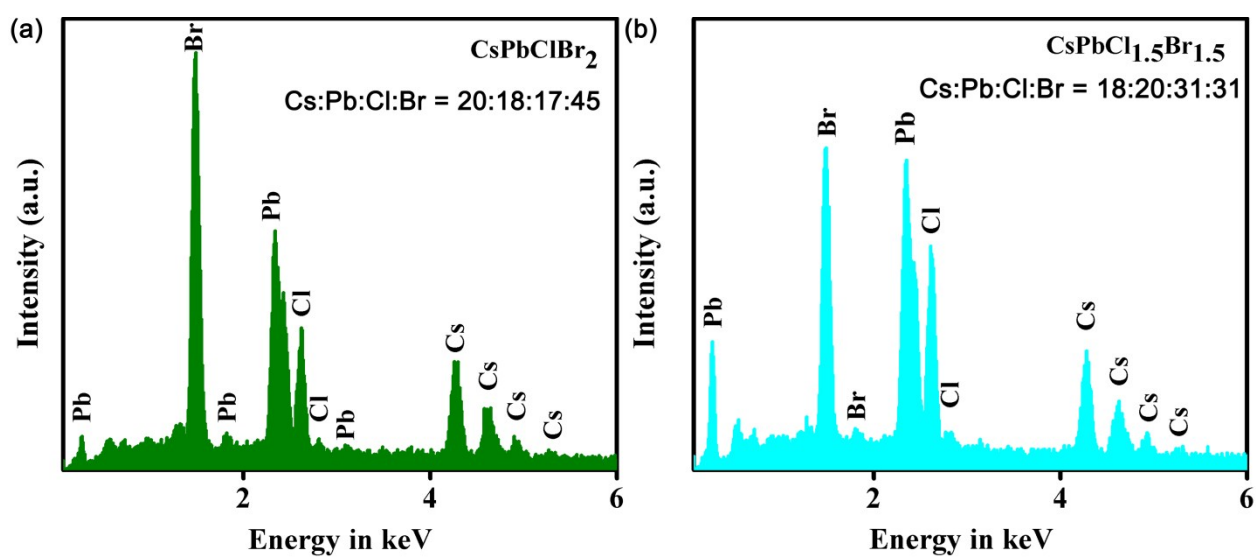


Figure S2: EDX spectra of the (a) CsPbClBr_2 (b) $\text{CsPbCl}_{1.5}\text{Br}_{1.5}$.

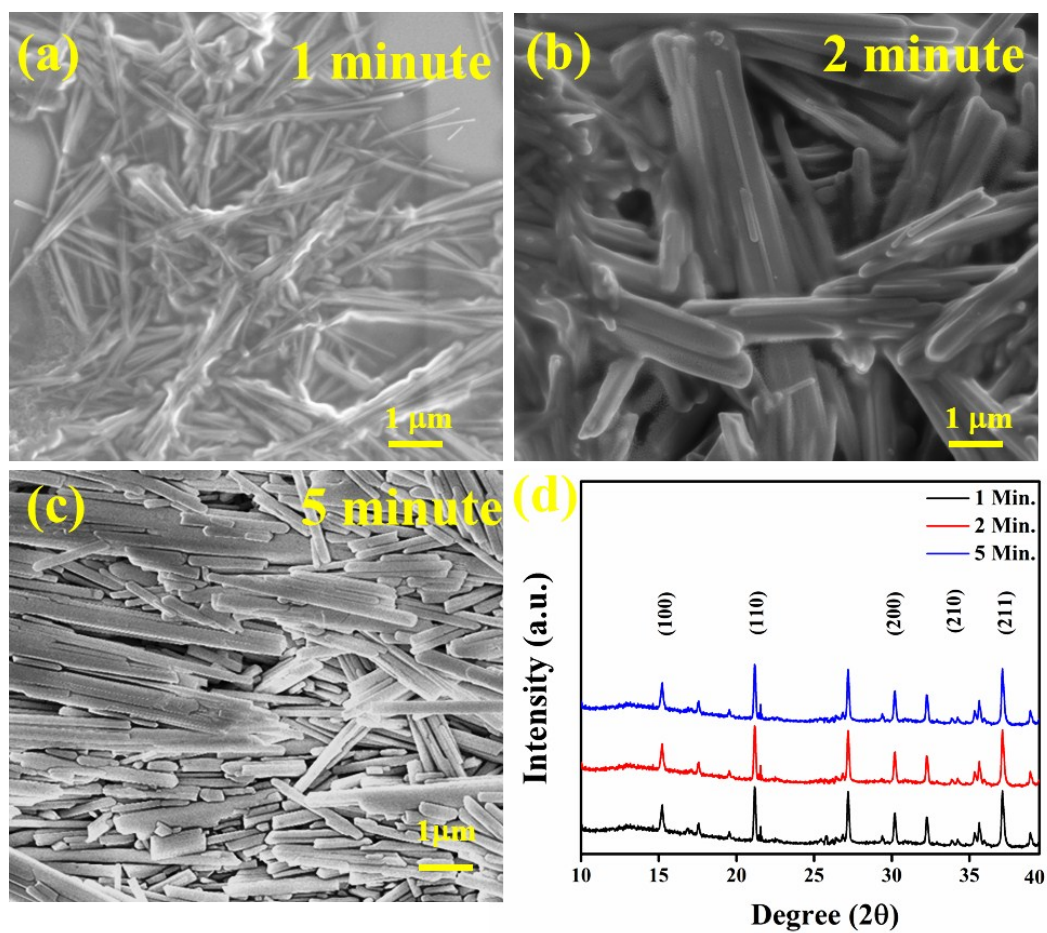


Figure S3: FESEM images showing structural evolution of CsPbI₃ sample with different time (a, b, c); Corresponding XRD pattern of the samples (d)

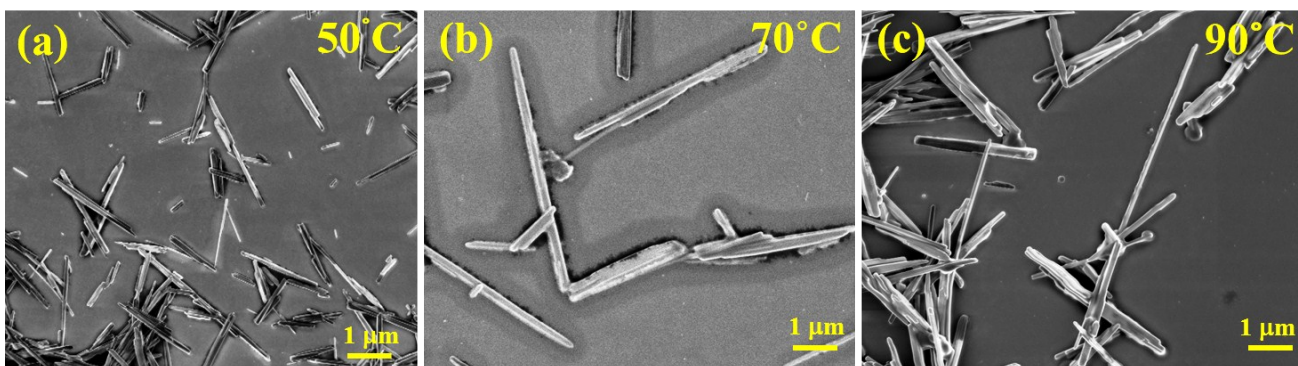


Figure S4: FESEM images of CsPbI₃ sample at different growth temperature

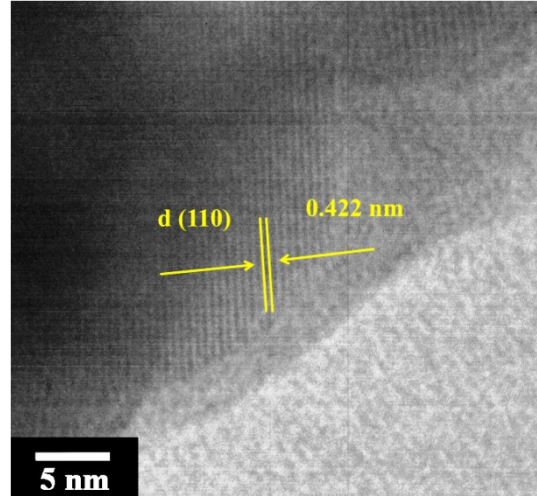


Figure S5: HRTEM image of CsPbBr_{1.5}I_{1.5} sample

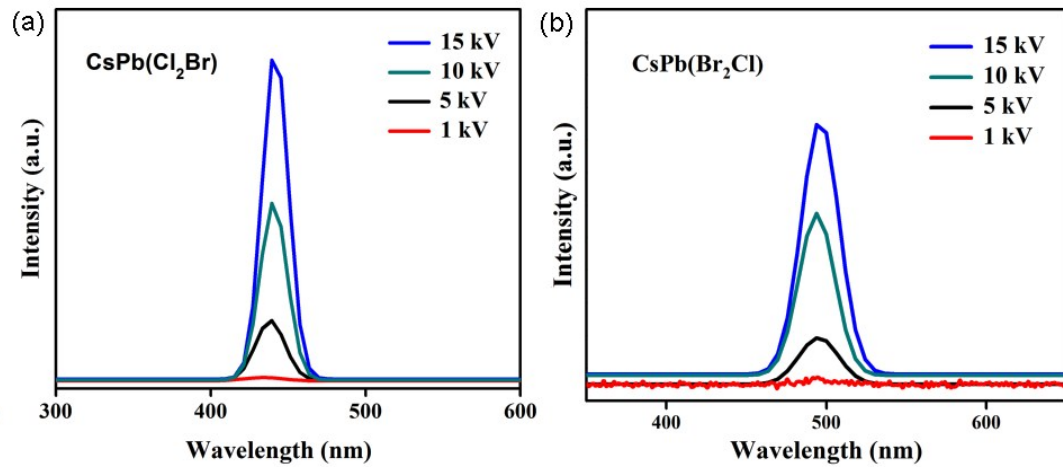


Figure S6: Accelerating voltage varied CL spectra of the (a) CsPbCl₂Br (b) CsPbBr₂Cl

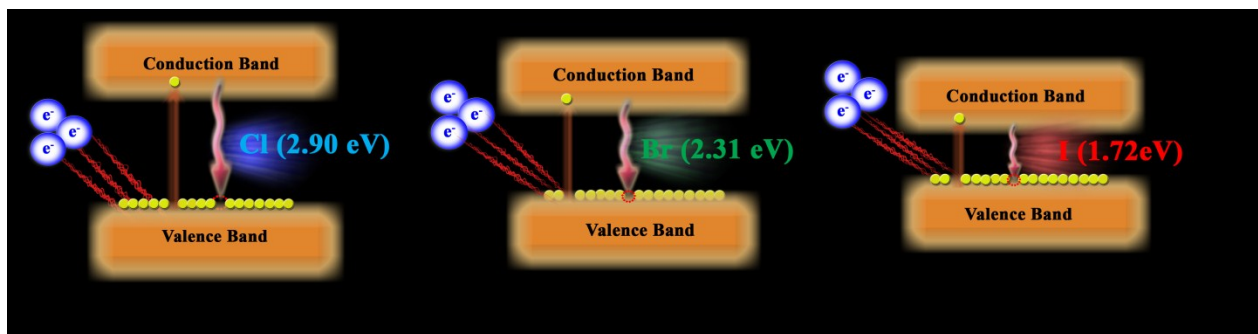


Figure S7: schematic illustration of electron-hole recombination in CsPbCl_3 , CsPbBr_3 and CsPbI_3 samples

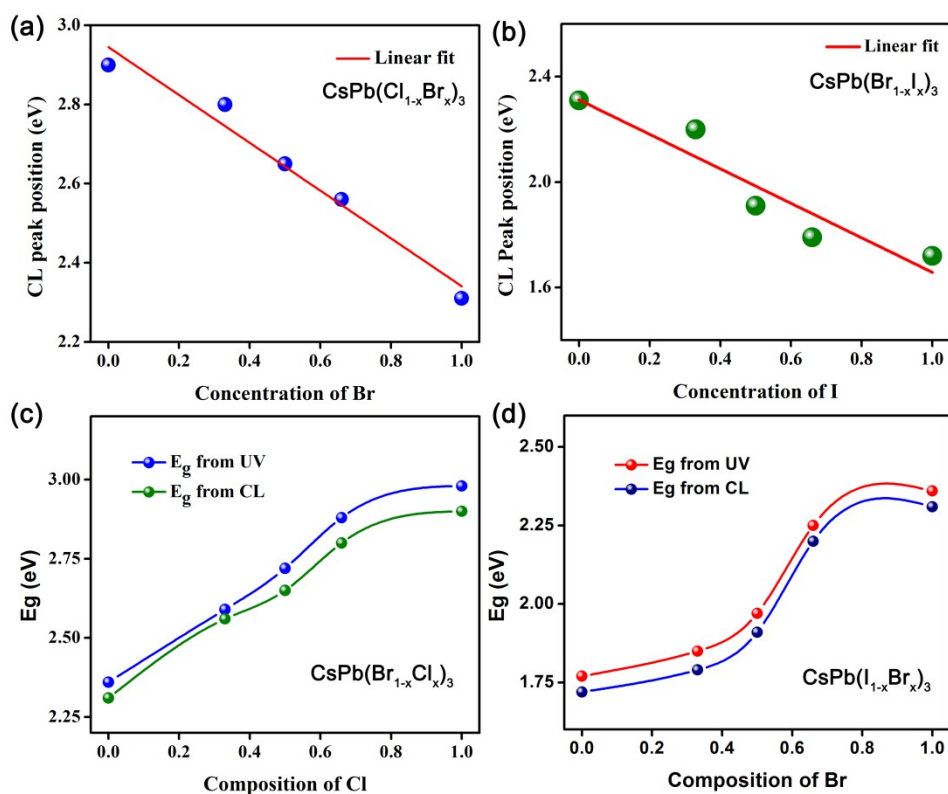


Figure S8: (a) Variation of CL peak position of $\text{CsPb}(\text{Cl}_{1-x}\text{Br}_x)_3$ samples with bromine concentration; (b) variation of CL peak position of $\text{CsPb}(\text{Br}_{1-x}\text{I}_x)_3$ with iodine concentration; variation of energy band gap estimated from UV-vis and CL spectra with increasing (c) chlorine concentration in $\text{CsPb}(\text{Cl}_{1-x}\text{Br}_x)_3$ and (d) bromine concentration in $\text{CsPb}(\text{I}_{1-x}\text{Br}_x)_3$.

Table S1: Crystal size and lattice strain of the synthesized samples.

Sample	Crystal size (nm)	Strain
CsPbCl ₃	62.71	0.0017
CsPbCl ₂ Br	92.40	0.0025
CsPbCl _{1.5} Br _{1.5}	65.68	0.0027
CsPbClBr ₂	107.44	0.0038
CsPbBr ₃	28.28	0.00261
CsPbBr _{1.5} I _{1.5}	76.15	0.00112
CsPbI ₃	58.48	0.00026

Table S2: Elemental composition of the synthesized samples.

Composition (Atomic %)	Cs	Pb	Cl	Br	I
CsPbCl ₃	19	21	60	-	-
CsPbCl ₂ Br	19	20	39	22	-
CsPbCl _{1.5} Br _{1.5}	18	20	31	31	-
CsPbClBr ₂	20	18	17	45	-
CsPbBr ₃	19	18	-	63	-
CsPbI ₃	18	20	-	-	62

Table S3: The lattice parameters of the optimized CsPbCl₃, CsPbBr₃ and CsPbI₃ unit cell

System	a (Å)	b (Å)	c (Å)
CsPbCl ₃	7.973	11.355	7.916
CsPbBr ₃	8.244	11.735	8.198
CsPbI ₃	8.906	12.665	8.819

Table S4: Comparison of PL quantum yield (QY) results of CsPbX₃ nanoforms available in literature

Type of CsPbX₃ nanostructure	PL QY in literature	Reference
CsPbBr ₃ Quantum Dot	70%	8
CsPbBr ₃ quantum Dot	27%	9
CsPbBr ₃ nano-platelet	19%	
CsPbBr ₃ nanorod	34%	
CsPbBr ₃ nanowire	29%	
CsPbBr ₃ quantum Dot	68%	10
CsPbBr ₃ nano-crystal	50-90%	11
CsPbBr ₃ nano-crystal	50-85%	12
CsPbI ₃ quantum Dot	30%	13
CsPbX ₃ nanowires	10.8%	14
CsPbX ₃ 1D architecture	37-48%	In this work

Reference

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