Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Synthesis of All-Inorganic $CsPb_2Br_5$ Perovskite and Determination of Its Luminescence Mechanism

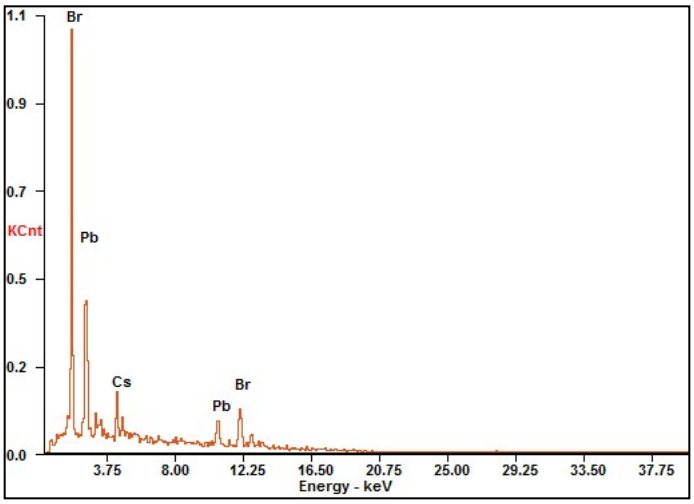
Jing Li, [a] Huijie Zhang, [a] Song Wang, [b] Debing Long, [a] Mingkai Li, [a] Yizhong Guo, [a] Zhicheng Zhong, [b] Kaifeng Wu, [c] Duofa Wang,*, [a] and Tianjin Zhang*, [a]

a Hubei Collaborative Innovation Center for Advanced Organic Chemical Materials, Key Laboratory of Green Preparation and Application for Materials, Ministry of Education, Hubei Provincial Key Laboratory of Polymers, Department of Materials Science and Engineering, Hubei University, Wuhan 430062, People's Republic of China

b Hubei Key Laboratory of Low Dimensional Optoelectronic Materials and Devices, Hubei University of Arts and Science, Xiangyang, Hubei 441053, China

c Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 457 Zhongshan Road, Dalian 116023, China

*E-mail:duofawang@hotmail.com, zhangtj@hubu.edu.cn



Element	*Wt%*	*At%*
BrL	45.15	65.40
PbM	42.16	23.55
CsL	12.69	11.05

Figure S1. Energy dispersive X-spectroscopy of $CsPb_2Br_5$. The ratio of each element is listed in the table.

Table S1. Total energy of unit cell for each reactant and the resultant chemical equation:

$$CsOH + 3PbBr_2 \longrightarrow CsPb_2Br_5 + Pb(OH)Br$$

The total energy of each materials is calculated based on the optimized structure using DFT. The change of the total energy is obtained by the difference between the products and the reactants.

	CsOH	**$PbBr_2$**	**$CsPb_2Br_5$**	**Pb(OH)Br**
Total energy (Et)	-386.66121413Ry	-1032.20505769Ry	-2505.07266819Ry	-978.53862569Ry

$$\Delta Et = Et_{CsPb2Br5} + Et_{Pb(OH)Br} - Et_{CsOH} - 3Et_{PbBr2} = -0.33507975Ry \approx -4.559\ ev$$

Movie S1. Movie S1.mp4