Organic Cation Engineering and its Effect on Distortion in 2D Halide Perovskites

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Abstract: Engineering of organic cation in 2D perovskite halide has gained attention in search of highly stable material with better structural tunability and optoelectronic properties. Degree of octahedral distortion is one such criteria that needs to be taken in account for better understanding of these properties.
The present work will show a systematic study of degree of distortion with increase in organic cation chain length. With the introduction of organic cation in a non-distorted 3D perovskite $Cs_2AgBiBr_6$, the single crystal XRD of $A'_4AgBiBr_8$ (Where A' is PA-Propylammonium, BA-Butylammonium and HA-Heptylammonium) showed dimensional reduction to 2D perovskite and significant inter and intra octahedral distortion. This degree of distortion has been quantified as a measure of bond length and bond angle variations.[1][2] Furthermore the impact of this distortion on optoelectronic properties and applications has been studied which will help the research community to choose the desired organic cation for their research.

REFERENCES

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[3] L. Mao, S. M. L. Teicher, C. C. Stoumpos, R. M. Kennard, R. A. Decrescent, G. Wu, J. A. Schuller, M. L. Chabinyc, A. K. Cheetham and R. Seshadri, *J. Am. Chem. Soc.*, **141** (2019), 19099–19109.

FIGURES

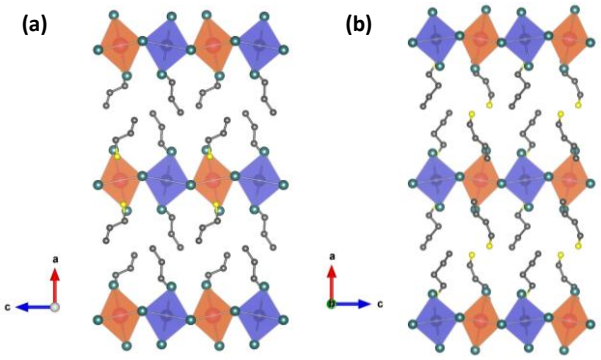

Figure 1: Crystal structure of 2D double perovskite (a) $PA_4AgBiBr_8$[3] at 293 K and (b) $BA_4AgBiBr_8$ at 298 K.

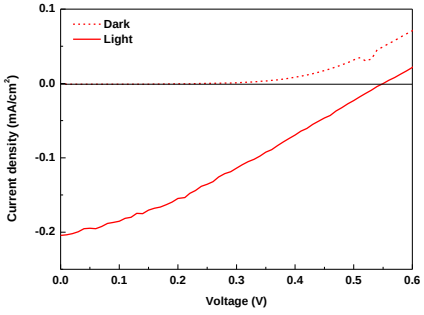

Figure 2: J-V curves of a $BA_4AgBiBr_8$ cell measured in the dark and light conditions.