

TEM Characterization of the Edges of CsPb₂Br₅ Perovskite Crystals

Hector A. Calderon¹, Francisco Robles-Hernandez,² Yanan Wang,^{3,4} Chong Wang,^{5,4} Xinghua Su,^{6,4}, Viktor G. Hadjiev,^{7,8} Yizhou Ni,^{7,9} Md Kamrul Alam,¹⁰ Yan Yao,^{4,7,10} Yu Yang,⁵ Shuo Chen,^{7,9} Zhifeng Ren,^{7,9} Zhiming Wang,³ Jiming Bao^{4,3,10}.

- ¹ Instituto Politecnico Nacional, ESFM, Depto. Física, CDMX, Mexico 07338.
- ² Mechanical Engineering Technology, The University of Houston, Houston, TX 77204, USA.
- ³ Inst. of Fund. Frontier Sci., U. of Electronic Science and Technology, Sichuan 610054, China.
- ⁴ Dep. of Electrical and Computer Engineering, University of Houston, Houston, Texas 77204, USA
- ⁵ Inst. of Optoelectronics, School of Mat. Sci. and Eng., Yunnan University, Kunming, 650091, China.
- ⁶ School of Materials Science and Engineering, Chang'an University, Xi'an, Shaanxi 710061, China.
- ⁷ Texas Center for Superconductivity, University of Houston, Houston, TX 77204, USA.
- ⁸ Department of Mechanical Engineering, University of Houston, Houston, TX 77204, USA.
- ⁹ Department of Physics, University of Houston, Houston, Texas 77204, USA.
- ¹⁰ Materials Science & Engineering, University of Houston, Houston, Texas 77204, USA.

Edges of CsPb₂Br₅ microplates have been characterized by low dose transmission electron microscopy together with energy dispersive spectroscopy measurements. CsPb₂Br₅ is a water resistant perovskite similar in character to CsPbBr₃ but with a two dimensional Pb-Br framework separated by Cs layers. These two compounds can coexist at the nanoscale forming nanocomposites or core shell arrangements that give rise to stable photoluminescence (PL). Nevertheless the PL properties of the CsPb₂Br₅ have been under controversy, some reports indicate a strong visible PL while others give inherent PL inactivity. In this work, clean CsPb₂Br₅ are synthesized through a simple water induced phase transformation from CsPbBr₃ to reduce potential chemical contamination. CsPbBr₃ powders are first synthesized using a modified method by mixing 0.5 M Pb(CH₃COO)₂·3H₂O and 1 M CsBr in 48% HBr solution at room temperature. CsPb₂Br₅ can then be synthesized by dropping CsPbBr₃ micro-cubes in water (20-50 times more water in mass) at room temperature. Atomically flat CsPb₂Br₅ microplatelets are prepared to distinguish edge photoluminescence from body emission and to prove that single crystal CsPb₂Br₅ is a two-dimensional wide bandgap semiconductor. Full details of the physical characterization are given elsewhere [1, 2].

Figure 1 shows phase images of a typical edges on the microplatelets at atomic resolution. The phase image is determined from an exit wave reconstruction (EWR) procedure that involves 40 experimental images at different defoci (MacTempass ®). The TEAM 0.5 electron microscope is used to acquire the experimental images at a dose rate of 20 e⁻/Å²s. Both images in Fig. 1 show three different areas with distinctive material phases: near the edge the phase CsPbBr₃ can be identified (I), the phase CsPb₂Br₅ is located at the farther end (III) and into the bulk of the sample and finally a mixture of phases is imaged in the intermediate region (II). The spatial distribution of phases is better appreciated by using a Fourier transform analysis as that shown in Fig. 2. Apparently the region near the surface (I) forms during the synthesis procedure in connection with chemical distribution of the involved elements. The inverse FFT in Fig. 2c shows patches of the CsPbBr₃ inside the mixture region (II) and then the phase CsPb₂Br₅ becomes predominant in regions relatively far from the surface (III). EDS measurement confirm the chemical differences observed in atomic resolution phase images.

References:

[1] V. G. Hadjiev *et al*, submitted to Physical Review B (2018).

[2] Y. Wang *et al*, to be published.

[3] HAC acknowledges support from IPN (SIP, COFAA) for a sabbatical stay at the Molecular Foundry-LBNL. Work at the Molecular Foundry was supported by the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

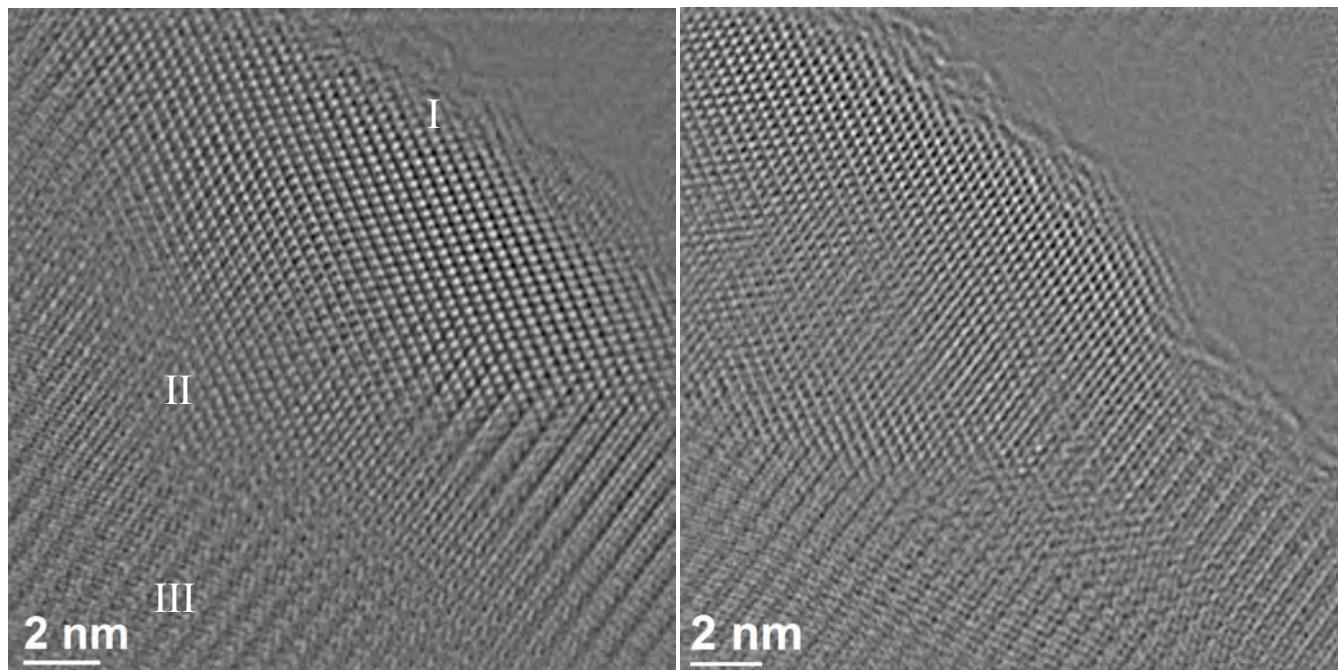


Figure 1. Typical phase images of edges in perovskite microplates. Three different regions are identified as CsPbBr_3 (I), a mixture of phases (II) and periodic CsPb_2Br_5 .

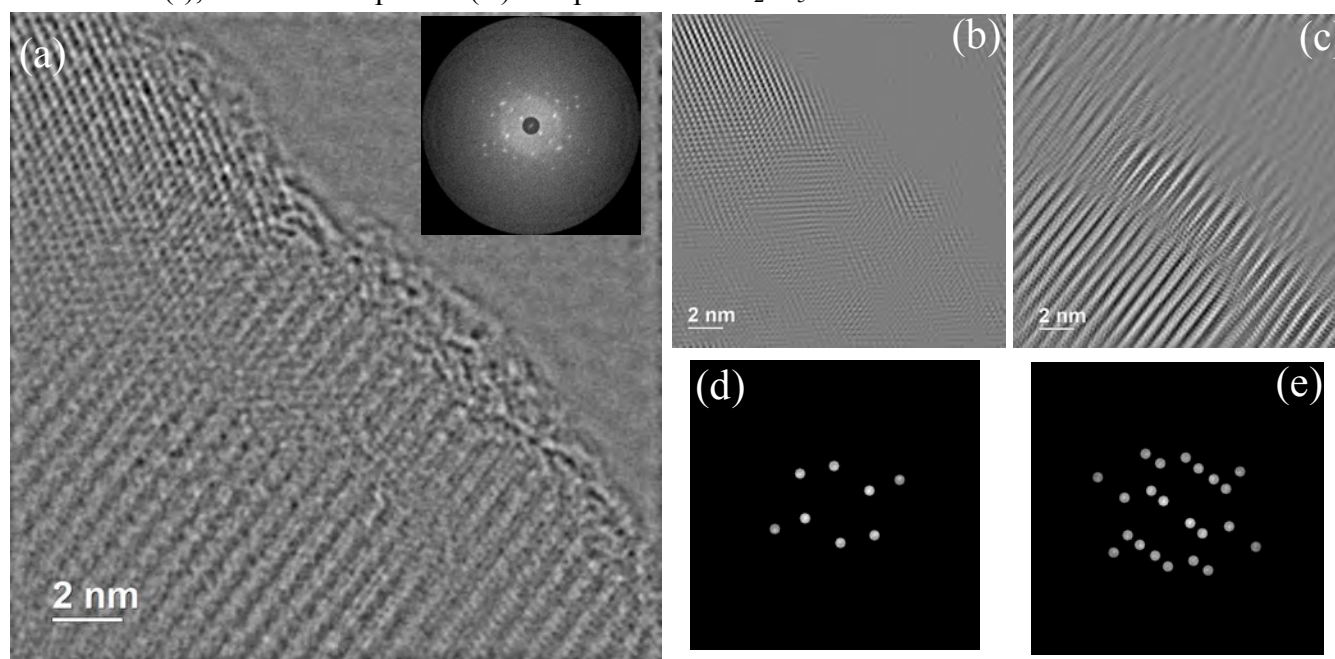


Figure 2. FFT Analysis of phase distribution. (a) Phase image and FFT. (b) IFFT showing distribution of CsPbBr_3 phase. (c) IFFT showing distribution of CsPb_2Br_5 . (d,e) Masks for IFFTs.