

# Liquid Water-Induced Growth of 1D morphology of $\text{CH}_3\text{NH}_3\text{PbI}_3$ Hybrid Perovskite

A. Bonadio, L. S de Oliveira, A. S. Polo, J. A. Souza  
*Universidade Federal do ABC, Santo André, SP, Brazil*

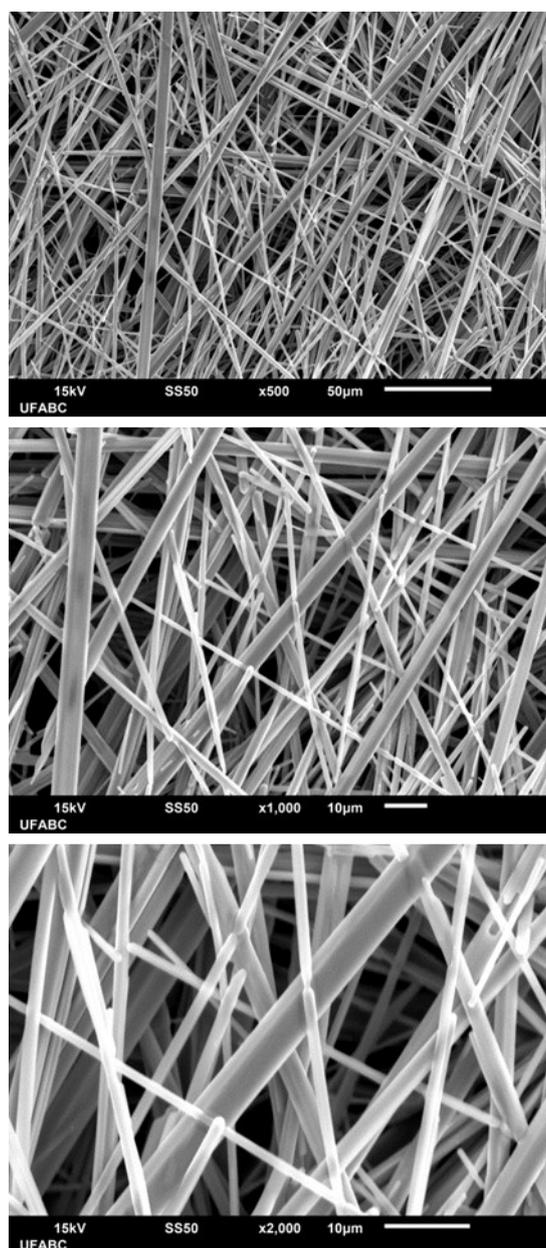


Fig. S1. Formation of monohydrate  $(\text{CH}_3\text{NH}_3 \cdot \text{H}_2\text{O})\text{PbI}_3$  microwires.

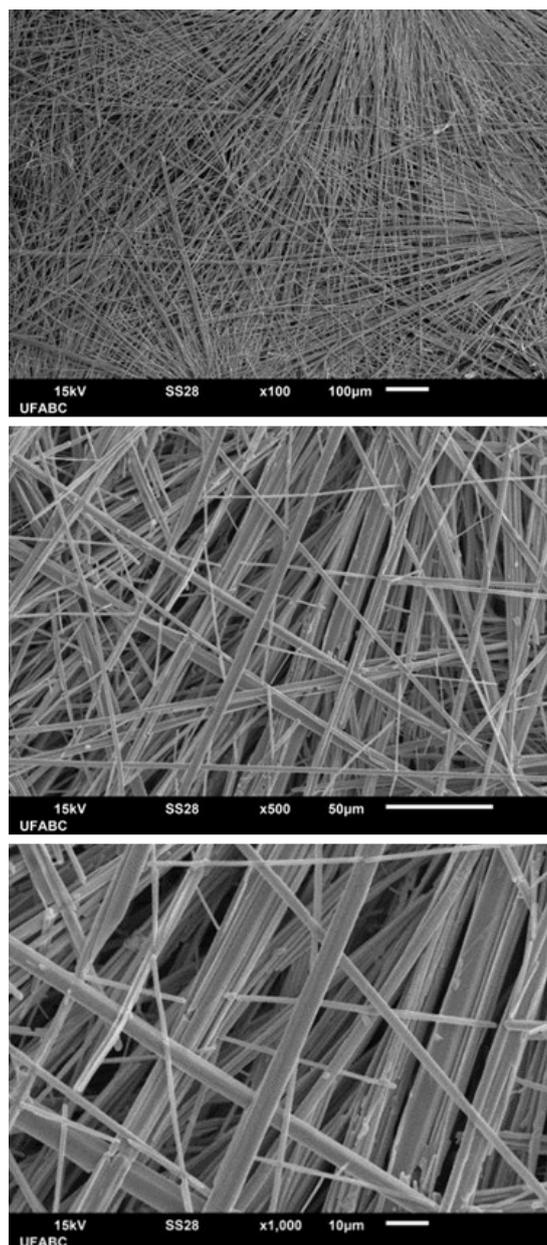


Fig. S2.  $\text{CH}_3\text{NH}_3\text{PbI}_3$  perovskite microwires formation after heat treatment of monohydrate species.

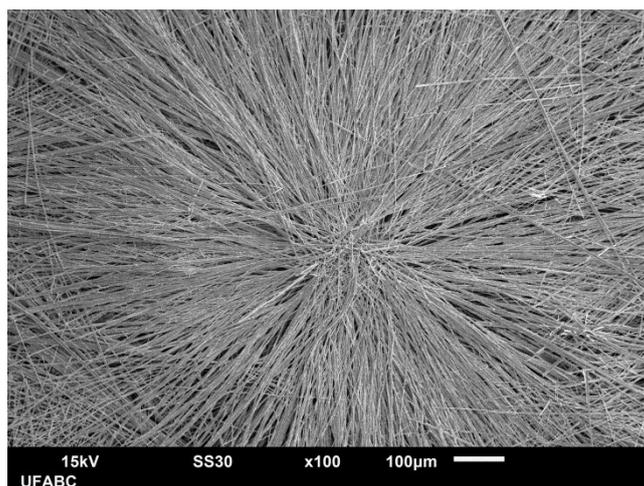


Fig. S3. Radial distribution of microwire array.

Varian 610 FT-IR Micro-spectrometer in the reflectance method for infrared measurements has been used to characterize our samples. Fig. S4 shows the infrared characterization of  $(\text{CH}_3\text{NH}_3 \cdot \text{H}_2\text{O})\text{PbI}_3$  and  $\text{CH}_3\text{NH}_3\text{PbI}_3$  samples. Table S1 summarizes the assignment and peak positions of vibrational modes. A difference can be seen between the two IR spectra. We can see spectral shifts for three peaks in the region of 900-1300  $\text{cm}^{-1}$  by comparing the two spectra. In addition, the appearance of the band at 1520  $\text{cm}^{-1}$  for  $\text{H}_2\text{O}$  bend peak is present only in the monohydrate compound. When the monohydrate is subsequently dried, the band assigned to water disappear, as we can see in  $\text{CH}_3\text{NH}_3\text{PbI}_3$  spectra. The  $\text{CH}_3\text{NH}_3\text{PbI}_3$  spectra is nearly identical to those reported before [1, 2].

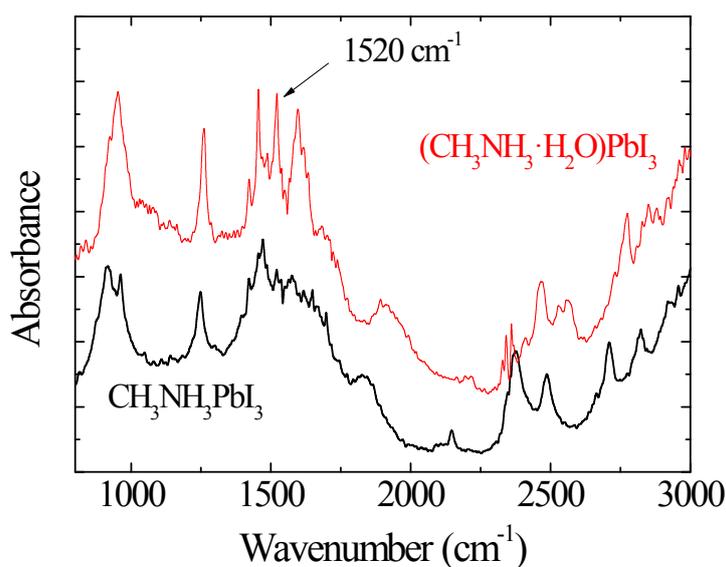


Figure S4. Infrared characterization of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  and  $(\text{CH}_3\text{NH}_3 \cdot \text{H}_2\text{O})\text{PbI}_3$  samples.

Table S1. Measured Vibrational Modes of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  and  $(\text{CH}_3\text{NH}_3 \cdot \text{H}_2\text{O})\text{PbI}_3$  samples.

IR band assignment	$\text{CH}_3\text{NH}_3\text{PbI}_3$ ( $\text{cm}^{-1}$ )	$(\text{CH}_3\text{NH}_3 \cdot \text{H}_2\text{O})\text{PbI}_3$ ( $\text{cm}^{-1}$ )
$\text{CH}_3\text{-NH}_3^+$ rock	916	923
$\text{CH}_3\text{-NH}_3^+$ rock	960	951
$\text{CH}_3\text{-NH}_3^+$ rock	1247	1260
$\text{CH}_3$ bend	1422	1421
$\text{CH}_3\text{-NH}_3^+$ bend	1453	1471
$\text{H}_2\text{O}$ bend		1520
$\text{NH}_3^+$ bend		1595

The energy dispersive spectroscopy (EDS) spectrum of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  microwires (Fig. S5) is presented in Fig. S6. The EDS spectrum shows the presence of Carbon, Nitrogen, Oxygen, Lead and Iodide. Carbon and Oxygen may be attributed to the carbon tape and impurities of the substrate used for this measurement, respectively. We can roughly approximate the ratio of Pb and I in the molecular formula to 1Pb:3I, accordingly to Table S2. However, it is hard to make this approximation for the organic part due to the possible inconsistent values for Carbon and Oxygen.

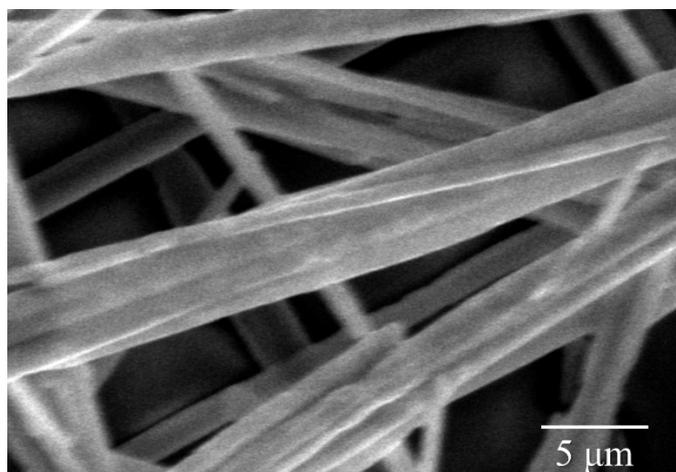


Figure S5. SEM image of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  microwires.

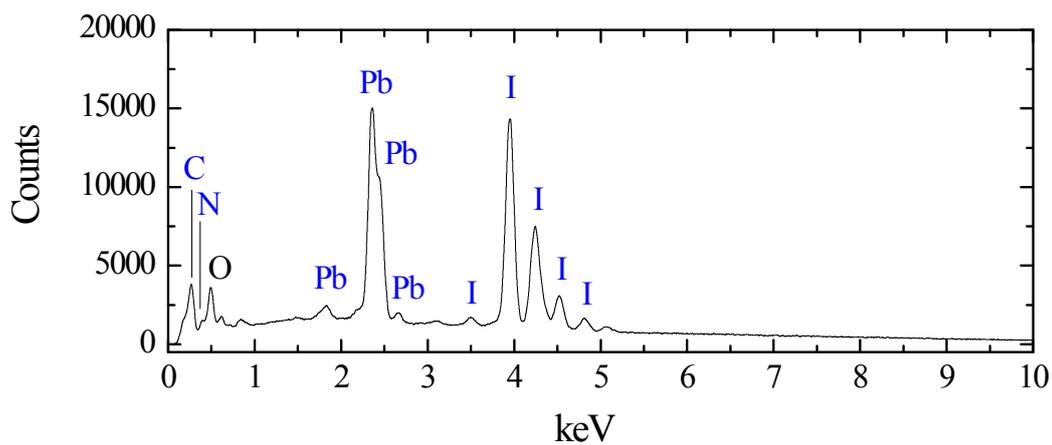
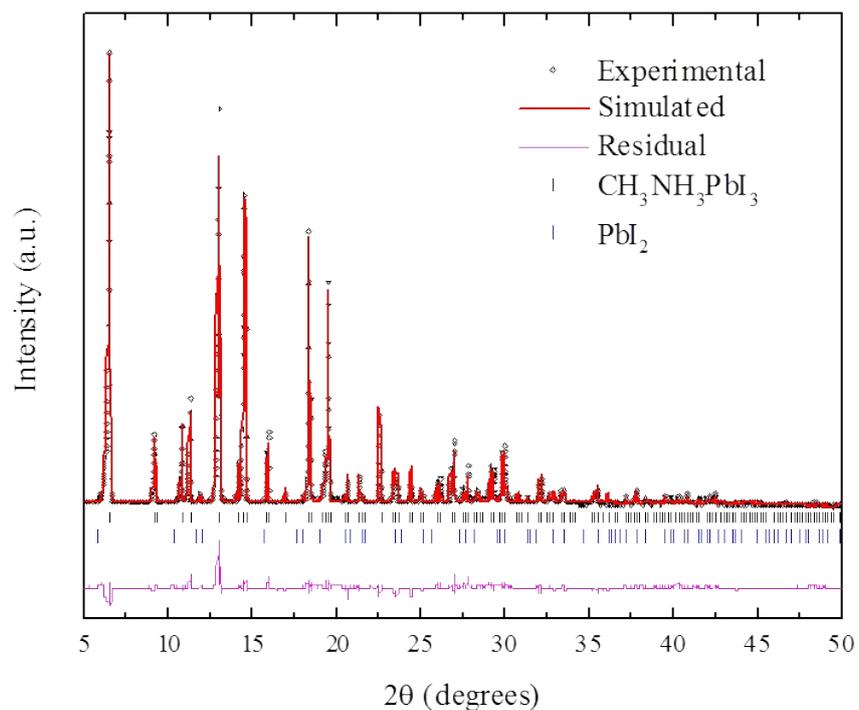


Figure S6. Energy Dispersive spectroscopy (EDS) spectra of  $\text{CH}_3\text{NH}_3\text{PbI}_3$  microwires.

Table S2. Percentage of elements present in the  $\text{CH}_3\text{NH}_3\text{PbI}_3$  sample.

C (%)	O (%)	N (%)	Pb (%)	I (%)
40.39	3.11	0.43	43.88	12.19

### Crystal Structure Report for $\text{CH}_3\text{NH}_3\text{PbI}_3$



<b>Chemical formula</b>	CH <sub>3</sub> NH <sub>3</sub> PbI <sub>3</sub>
<b>Formula weight</b>	619.96 g/mol
<b>Temperature</b>	300 K
<b>Wavelength</b>	0.7107 Å
<b>Crystal system</b>	Tetragonal
<b>Space group</b>	I 4 / m c m
<b>Unit cell dimensions</b>	a = b = 8.850 Å      α = β = γ = 90 ° c = 12.637 Å
<b>Volume</b>	989.296 Å <sup>3</sup>
<b>%Wt</b>	99.4%

<b>Chemical formula</b>	PbI <sub>2</sub>
<b>Formula weight</b>	461.01 g/mol
<b>Temperature</b>	300 K
<b>Wavelength</b>	0.7107 Å
<b>Crystal system</b>	Trigonal
<b>Space group</b>	P -3 m 1
<b>Unit cell dimensions</b>	a = b = 4.544 Å      α = β = γ = 90 ° c = 6.970 Å
<b>Volume</b>	124.643 Å <sup>3</sup>
<b>%Wt</b>	0.6%

### Crystal Structure Report for (CH<sub>3</sub>NH<sub>3</sub>·H<sub>2</sub>O)PbI<sub>3</sub>

<b>Chemical formula</b>	(CH <sub>3</sub> NH <sub>3</sub> ·H <sub>2</sub> O)PbI <sub>3</sub> b
<b>Formula weight</b>	637.97
<b>Temperature</b>	300 K
<b>Wavelength</b>	0.7107 Å
<b>Crystal system</b>	Monoclinic
<b>Space group</b>	P 1 21/m 1
<b>Unit cell dimensions</b>	a = 10.525(4) Å      α = 90 ° b = 4.668(1) Å      β = 101.195(3) ° c = 11.176(8) Å      γ = 90 °
<b>Volume</b>	538.707(9)Å <sup>3</sup>

---

[1] Chen, J.; Mo, Z. H.; Yang, X.; Zhou, H. L.; Gao, Q. *Chem. Commun.*, 2017, **53**, 6949-6952.

[2] Zhu, Z.; Hadjiev, V.; Rong, Y.; Guo, R.; Cao, Bo.; Tang, Z.; Qin, F.; Li, Y.; Wang, Y.; Hao, F.; Venkatesan, S.; Li, W.; Baldelli, S.; Guloy, A. M.; Fang, H.; Hu, Y.; Yao, Y.; Wang, Z.; Bao, J. *Chem. Mater.*, 2016, **28**, 7385–7393.