

## BOISE STATE UNIVERSITY

## Abstract

Recent advances in the efficiency of hybrid perovskite solar cells have motivated extensive research aimed at increasing stability with respect to humidity and light.<sup>[3],[1]</sup> It is known that altering the chemistry of the perovskite crystal can alter the lattice structure, and in turn, stability.<sup>[2],[1]</sup> In order to fabricate more stable methylammonium lead (II) iodide (MAPbI<sub>3</sub>) cells, a series of precursor solutions was created by substituting increasing amounts of thiocyanate (SCN) for iodide following the stoichiometric form MAPbI<sub>(3-x)</sub>(SCN)<sub>x</sub>. While no working devices were fabricated due to the suspected decomposition of the p-type layer, X-ray diffractometry was ultimately used to characterize the changes in the crystal lattices.



MAPbI<sub>2</sub> Crystal Structure<sup>[4]</sup> Substitution at the X-site, <sup>[-</sup> and SCN<sup>-</sup> have similar effective ionic radii<sup>[1]</sup>



# Methods

#### Fabrication:

- Ambient humidity conditions
- Substrate cleaning:
- sonicated in acetone
- ozone/UV (improve coverage) • Spin-coating:
- p-type: nickel oxide
- MAPbI<sub>(3-x)</sub>(SCN)<sub>x</sub>
  - Solvent: dimethylformamide
  - chlorobenzene quench<sup>[5]</sup>
- n-type: PCBM (phenyl C<sub>61</sub> butyric acid methyl ester)

- Sputter-coated Al electrodes • Instrument: AJA Orion 5 **Characterization:**
- SEM
- Instrument: FEI Teneo • XRD
  - Instrument: Rigaku Miniflex 600
  - Software: GSAS-II<sup>[6]</sup>

## References

- [3] Bai, S, et al. Reproducible Planar Heterojunction Solar Cells Based on One-Step Solution-Processed Methylammonium Lead Halide Perovskites, DOI: 10.1021/acs.chemmater.6b05159 Chem. Mater. 2017, 29, 462–473(2017). [4] Jin Cui, et al 2015 Sci. Technol. Adv. Mater. 16 036004
- [5] S. Paek, From Nano- to Micrometer Scale: The Role of Antisolvent Treatment on High Performance Perovskite Solar Cells Chem. Mater. 2017, 29, 3490-3498. [6] B.H. Toby & R.B. Von Dreele, J. Appl. Cryst. 46, 544-549 (2013)
- 7] Ben Mills, Public Domain, Structure calculated using HF/6-31G\* in Spartan '04 Student Edition. Image generated in Accelrys DS Visualizer.

# Hybrid Perovskite Solar Cells Erik Nordquist,\*,<sup>†</sup> Brad Kinney,<sup>†</sup> Rick Ubic<sup>†</sup> \* The College of Idaho <sup>†</sup> Boise State University









# Results

Cells were fabricated with the perovskite layer then characterized initially with scanning electron microscopy (SEM). Changes in the uniformity of coverage as the amount of SCN increased are shown below. It is clear that for x > 0.8, a different crystal structure forms. The figures below are paired as unmagnified optical pictures and SEM images.







#### Notes:

A: highly reflective surface, pure PbI<sub>2</sub> precursor B: apart from impurities, the surface appears very uniform C: very thin layer of a new phase (red) D: evidence of different crystal structure and poor coverage

[1] Ze Wang, et al. Stability of Perovskite Solar Cells: A Prospective on the Substitution of the A Cation and X Anion, Angew. Chem. Int. Ed. 2017, 56, – Angew. Chem. 2017, 129 [2] Tai, Q, et al. Efficient and stable perovskite solar cells prepared in ambient air irrespective of the humidity. Nat. Commun. 7:11105 DOI: 10.1038/ ncomms11105 (2016).

x = 0.2

## Contact

Erik.Nordquist@Yotes.CollegeofIdaho.edu



Conclusion

For lower concentrations of SCN in precursor solutions, the resulting perovskite phases seem to be mostly tetragonal, as in the base case of x = 0.0 where pure MAPbI<sub>3</sub> formed. Future work should aim to relate the SCN concentration to the stability of working devices, which could seed a model used to predict the effects of other anion substitutions. Furthermore, comparisons of the stability of devices made in controlled humidity should be made.





The XRD spectra were refined using GSAS-II<sup>[6]</sup> and fitted to published MAPBI, data. All three lattice parameters remain relatively constant for the tetragonal phase while 0.0 < x < 0.8. This could indicate that SCN is not altering the lattice size, or that it is not being incorporated at all. As the amount of SCN increased, a new orthorhombic phase emerged, shown in the x = 0.6 figure. Perovskite was not formed at the higher concentrations (x > 1.0), and these spectra were not analyzed further.

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