Scaling of All-Inorganic Perovskite Solar Cells through Improved Thermomechanical and Optoelectronic Stability

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Optoelectronic Properties

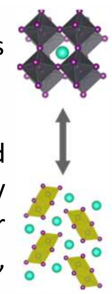
Thermomechanical Properties

Driving Question

In less than 80 minutes, enough sunlight's hits the earth's atmosphere to power the earth's energy needs for 1 year. **What is holding us back from using this energy?**

Background

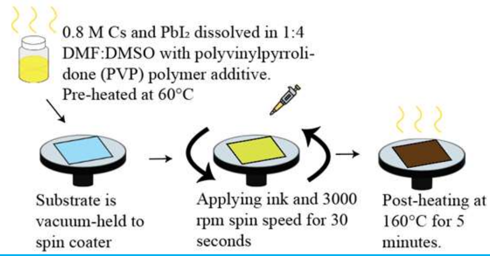
Perovskite solar cells (PSC) have the potential for low-cost processing and tunable band gaps. All-inorganic CsPbI3 is a type of high bandgap perovskite that is more compositionally and thermally stable in comparison to their organic counterparts, making it ideal for tandem cells. However, CsPbI3 has poor phase stability and requires high formation energy, resulting in poor performance and stability [1,3].

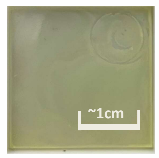


α-$CsPbI_3$, photoactive "black phase"

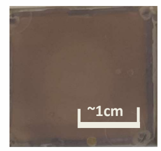
δ-$CsPbI_3$, non-photoactive "yellow phase"

[2]

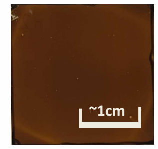




0% PVP, yellow phase



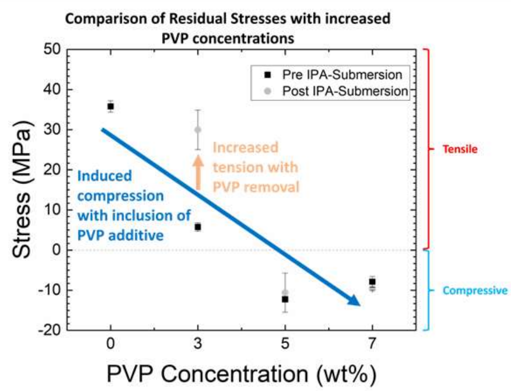
3.4% PVP, darkened, non uniform



6.5% PVP, ideal brown/black phase

Phase 1: Thermomechanical Properties

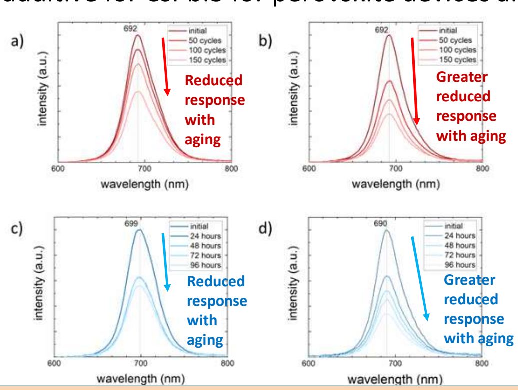
This study shows a stabilized phase and improved durability of all-inorganic CsPbI3 films through the polymer polyvinylpyrrolidone (PVP) as a precursor additive. PVP induces a desired compressive state and the removal of PVP is shown to affect low concentrations of PVP more significantly.



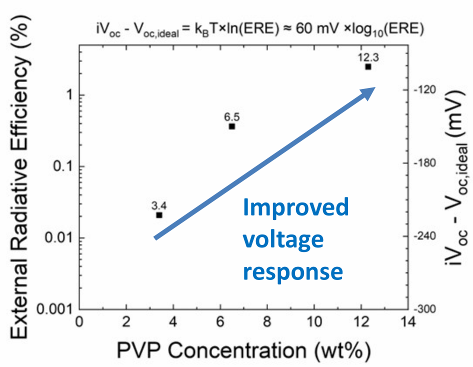
PVP Concentration	0%	3%	5%	7%
Pre-IPA Stress (MPa)	35.8	5.75	-12.25	-7.9
Post-IPA Stress (MPa)	---	29.97	-10.6	-9.63

Phase 2: Optoelectronic Properties

This research demonstrates the improved optoelectrical properties of photoluminescent (PL) and ionic properties of CsPbI3 under thermal aging and light exposure due to the polymer polyvinylpyrrolidone (PVP) as a precursor additive for CsPbI3 for perovskite devices and films



PL under thermal cycling with PVP a) kept, b) removed and light-induced aging with PVP c) kept, b) removed. Responses decrease more significantly under PVP removed.



ERE responses of varying concentrations. Higher responses are shown with larger PVP concentrations

Future Work

- Further study how optoelectronic properties evolve with ion concentration
- Further tune film residual stresses via additive engineering while optimizing optoelectronic properties.

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References

[1]Xiaoming Zhao et al., Accelerated aging of all-inorganic, interface-stabilized perovskite solar cells.*Science* **377**,307-310(2022).DOI:10.1126/science.abn5679

[2] "Exploring the black-to-yellow phase transformation mechanism of metal halide perovskites via machine learning potentials," Exploring the black-to-yellow phase transformation mechanism of metal halide perovskites via machine learning potentials | Center for Molecular Modeling, https://molmod.ugent.be/subject/exploring-black-yellow-phase-transformation-mechanism-metal-halide-perovskites-machine (accessed Nov. 3, 2023).

[3]Julian A. Steele et al., Thermal unequilibrium of strained black CsPbI3 thin films.*Science* **365**,679-684(2019).DOI:10.1126/science.aax3878

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