Solar Cells for Vehicle Surfaces: Tuning Halide Ion Concentration to Offset Bending Effects on Flexible Halide Perovskites Optoelectronics

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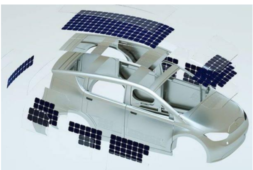
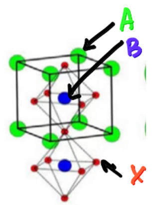
The findings

Why perovskites?



- Pioneering the future of clean energy, solar cells are setting new benchmarks and ensure environmental sustainability.
- ***Flexible halide perovskites:*** new class of solar cell materials that can be processed cheaply
- Excellent optoelectronic properties; improved efficiencies over commercial technologies
- Can be used for vehicle surfaces

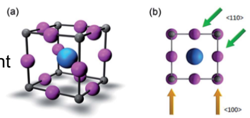
Understanding perovskites



Lead-based (Pb) Perovskites are defined by a general formula $APbX_3$, where 'A' is a cation, and 'X' is a halide anion

The crystal structure of perovskites allows chemical compositions (halide ion concentrations) to be altered, leading to ***tunable optoelectronic properties***: band gap energy, charge carrier mobility and thermal conductivity

Perovskite shows a complex response to strain due to different bond types in different directions. This provides another approach to tuning its optoelectronic properties



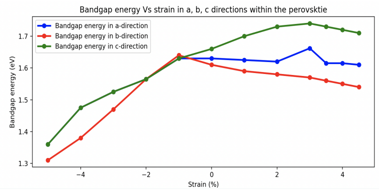
Research goals

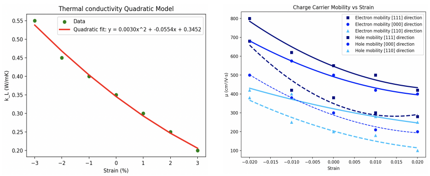
Determine how the curvature of bending affects the optoelectronic properties of a perovskite and the overall efficiency of a solar cell

Offset negative change by tuning halide ion concentration of a perovskite

Create models of a perovskite on a car surface, tuning the local halide ion concentration to offset the effects of curvature

To do this, we looked into growing perovskite single crystals, performing hyperspectral imaging to get PL spectra, THz for charge carrier mobility and thermal conductivity (not my data), DFT via Quantum Espresso for initial calculations, and Matlab & Python for summarising the graphs found and creating the models.



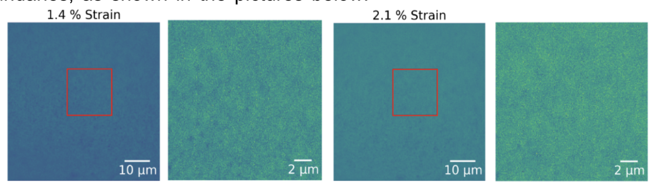


Bending creates a distortion within perovskite, shifting atomic orbitals of Pb atoms. This affects valence band maximum (VBM), so band-gap energy varies.

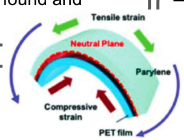
Compressive strain:

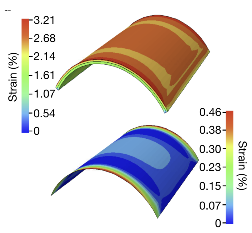
- Increases VBM (top figure)
- Decreases distance between perovskite and electrode, which increases the charge carrier mobility and thermal conductivity (bottom 2 figures)

Our results also agree with theoretically predicted and experimental results. Photobrightening was observed in the sample with an increase closer to the boundaries, as shown in the pictures below.



Strain Engineering

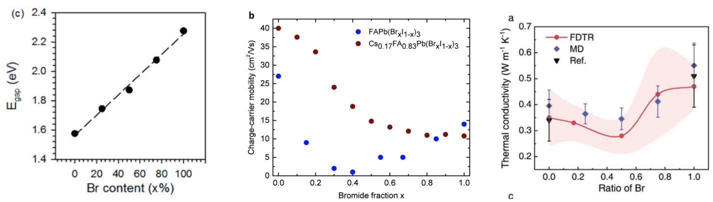




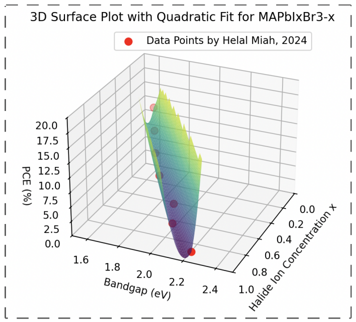
Internal and external strains:

- When a perovskite is bent, strain is induced.
- There is also initial strain within perovskite solar cell due to growth methods, interaction with other layers and a non-ideal Goldschmidt tolerance factor.
- These were calculated using MatLab PDEs and FEA

Compositional engineering



Big Picture: Improving Solar Cell Efficiency



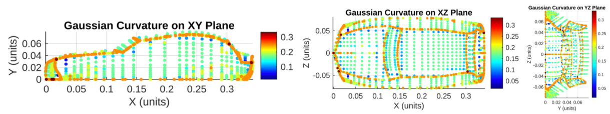
For a general model of a perovskite solar cell, we analyse the impact of strain and halide concentration on the power conversion efficiency.

Strain compensation strategies:

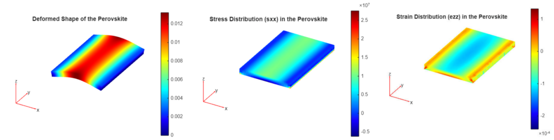
- Compatibility of thermal expansion coefficients of perovskite and other layers.
- Use nanowires to add an additional aspect of strain engineering.

Simulations

1) Programme created to extract the surface curvature of any car surface in .OBJ/ .STL files



2) Stress distributions within the perovskite layers under varying curvature were calculated

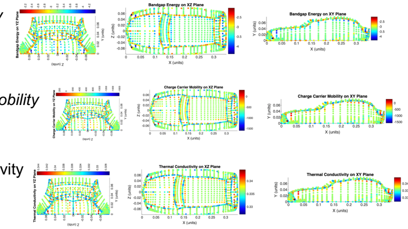


3) Changes in perovskite optoelectronic properties were mapped to the position within a perovskite surface

a) Band Gap Energy

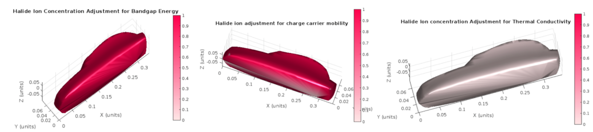
b) Charge Carrier Mobility

c) Thermal Conductivity



4) Properties optimised using relationships extracted from the graphs

5) Halide ion concentration needed to offset curvature-induced changes was found and mapped



Future directions and Applications

Perovskites can be used for wearable devices such as strain sensors and flexible displays. For a fuller picture, it would be crucial to investigate the stability of perovskites and look into their other optoelectronic properties during bending.

Acknowledgements

I am deeply grateful to Dr Claire Barlow overseeing this project, reviewing both the report and the poster and ensuring that I actually get things done.

Furthermore, I am thankful to Dr Miloš Dubajić and Capucine Mamak for helping with the measurements, explaining hyperspectral imaging and photo-induced halide separation like I am five and letting me use their samples. Additionally, I appreciate the input of Greg Chu with the substrates (despite that I thought OHP substrate was a file), and Aldric Goh & Dr Stephanie Adeyemo for introducing me to THz and helping get started with the project.