Development of a Fourth Generation Machine Learned Potential with Long-Range Flexible Charges for Two-Dimensional CsPbI Perovskites

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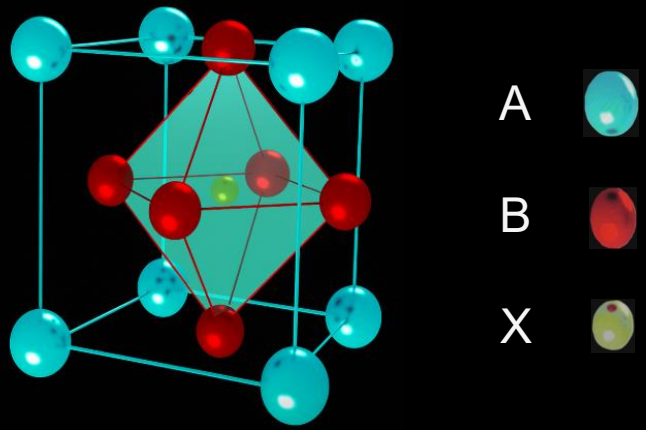
Perovskites

Tunable composition

Applications:
Solar cells to quantum computing

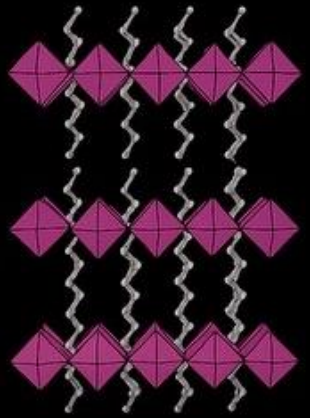
Low cost & lightweight

ABX_3 Structure

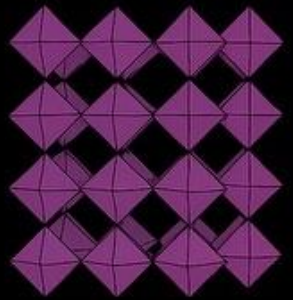


ABX_3 Structure

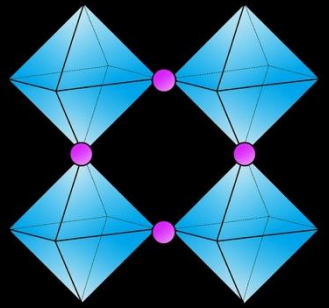
Why 2D Perovskites and CsPbI?



2D Perovskite

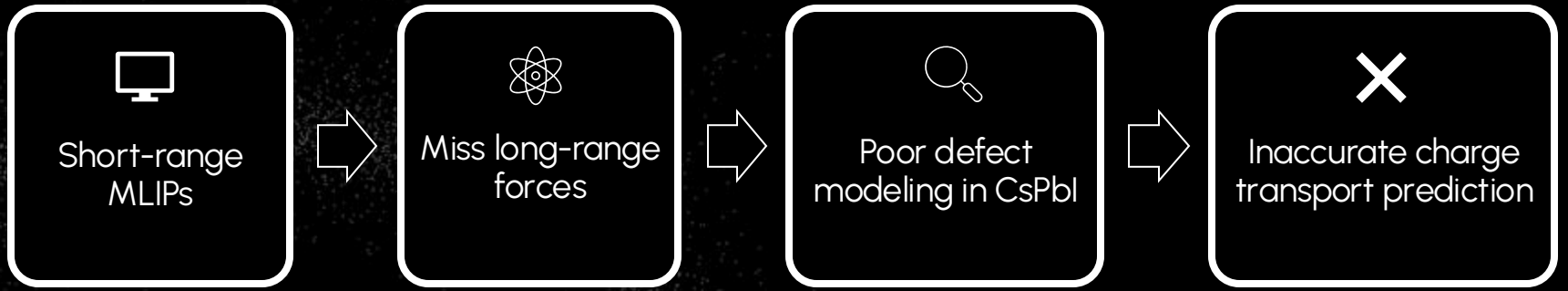


3D Perovskite



Cesium Lead Iodide (CsPbI)

The Modeling Problem



Why Machine Learning?

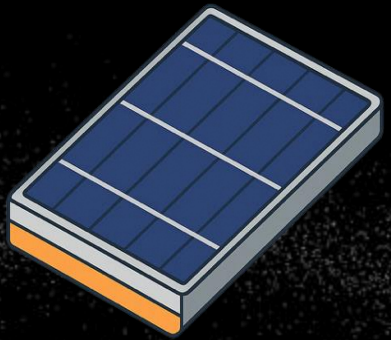
Density Functional Theory (DFT)

Accurate but computationally expensive

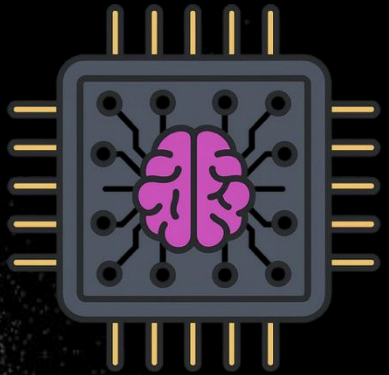
Machine-Learned Interatomic Potentials (MLIPs)

Accurate and faster

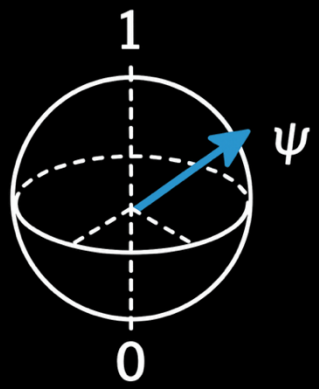
Why This Work Matters?



Solar Cells



Neuromorphic Computing Systems



Qubit

- Texas A&M University
- Los Alamos National Laboratory

The Proposed Architecture

Flexible machine-learning model to determine electronegativity

⇩

Generate a dataset of 2D CsPbI

⇩

Train a HIP-NN model to predict per-atom electronegativities

⇩

Train a second HIP-NN model to predict short-range energies and forces

⇩

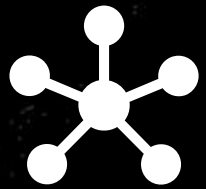
Combine both models

⇩

Validate the model against Density Functional Theory outputs

Theoretical Development

Literature reviews



Neural network architecture

Modeling pipeline

Computational Tools Utilized

Pymatgen

ASE
(Atomic Simulation Environment)

xTB
(Extended Tight Binding)

Next Steps

- Finalizing the Density Functional Theory dataset.
- Training the HIP-NN models for electronegativity and force prediction.
- Validating model performance.
- Simulate realistic atomic behavior.

Thank you