Molecular Dynamics Simulation Using Machine Learning interatomic potential for CsPbI3 perovskite

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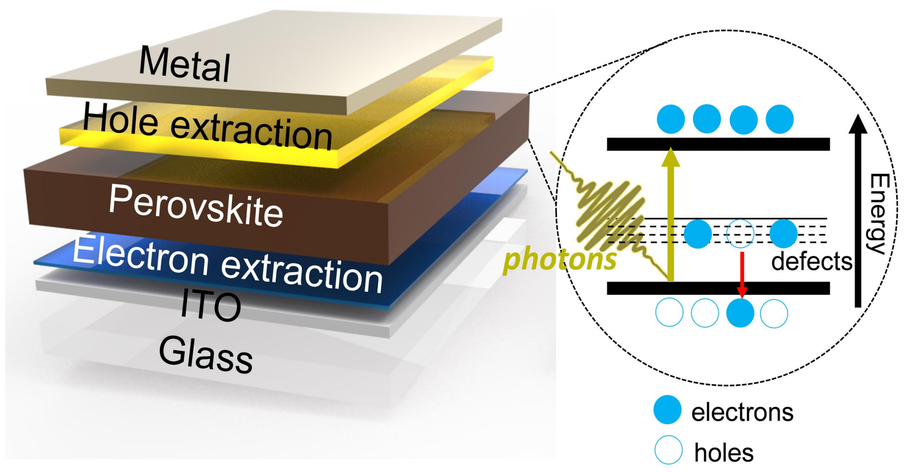
INTRODUCTION

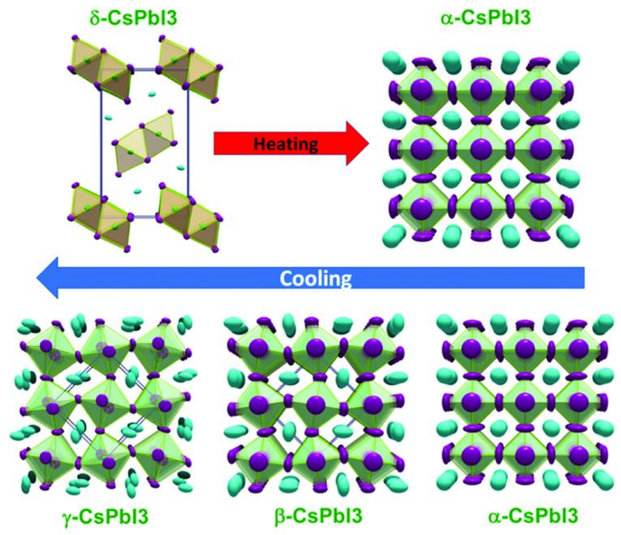
$CsPbI_3$ is a lead-halide perovskite with great potential for solar cells and optoelectronics.
It exhibits multiple structural phases driven by octahedral tilting, affecting its stability and performance.
Understanding its phase behaviour requires accurate modelling of these distortions.

AIMS

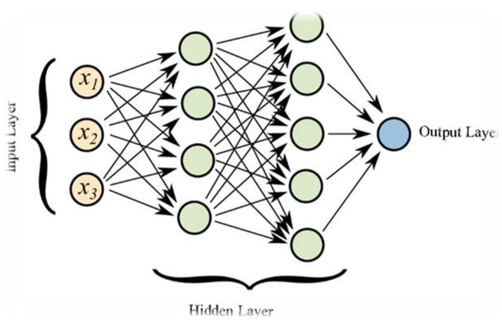
- Generate a high-quality dataset for accurate prediction of atomic forces and energies using machine learning techniques.
- Develop a predictive model capable of supporting MD simulations for perovskite materials.
- Perform MD simulations to investigate lattice dynamics and octahedral tilting behavior in perovskite structures.
- Facilitate structural analysis to support the design and optimization of perovskite solar cells

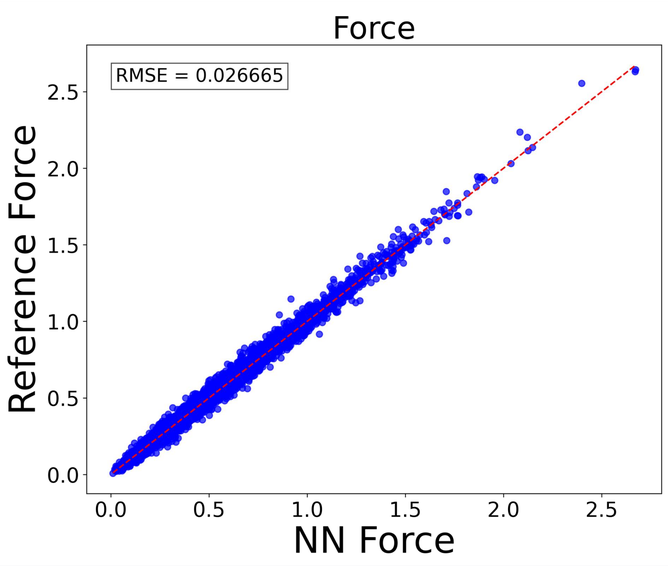


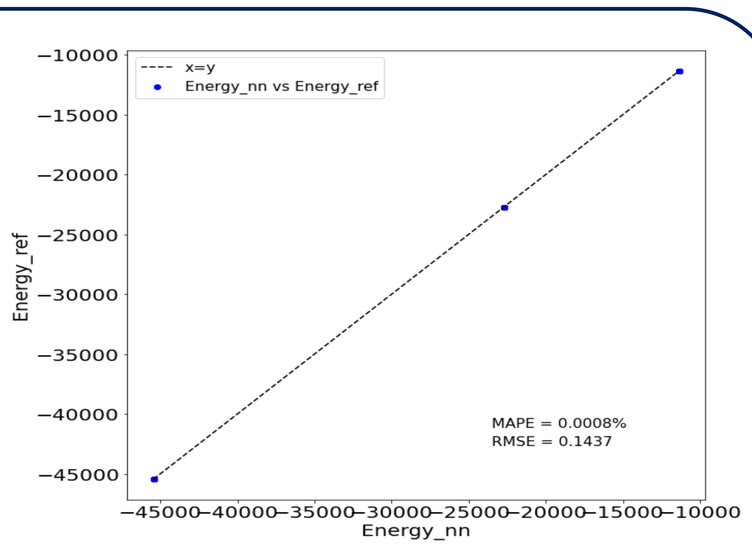
To generate the dataset, different phases of $CsPbI_3$—including cubic, tetragonal, orthorhombic, and the non-perovskite yellow phase—were sampled at various temperatures.

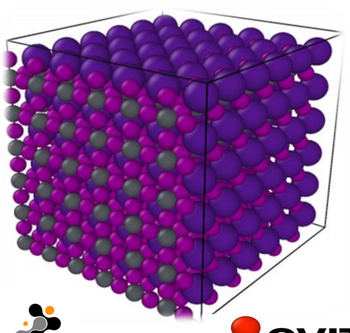


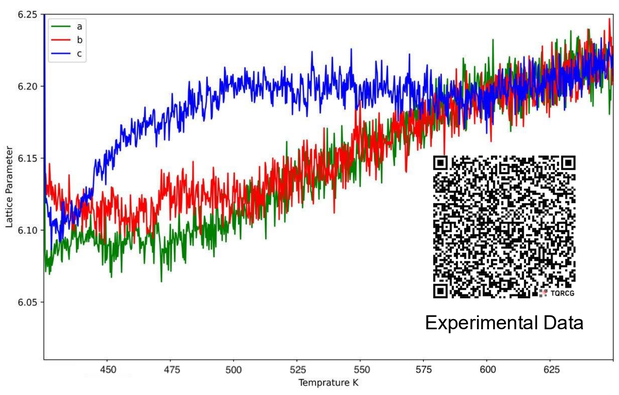
LATTE paper

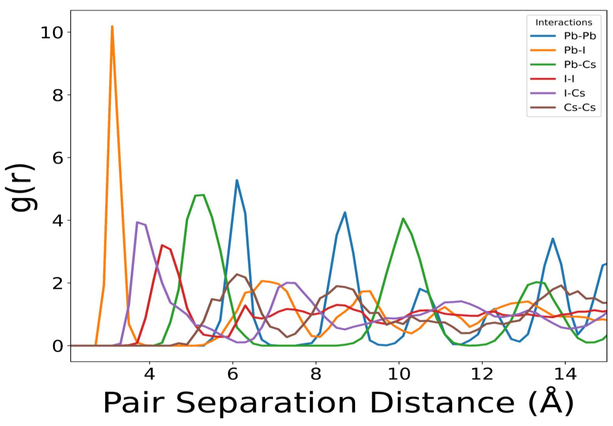


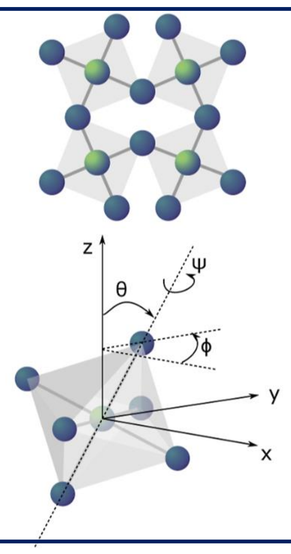


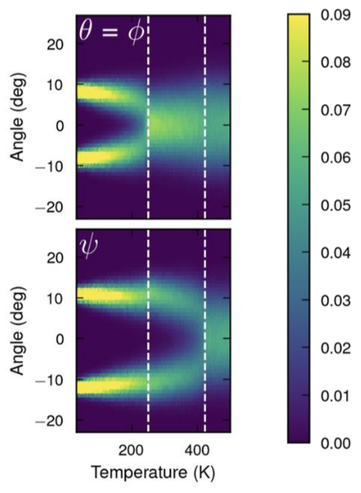












CONCLUSION

We developed a machine-learned interatomic potential using the LATTE framework to simulate the structural dynamics of $CsPbI_3$.
Key Achievements:

- Accurate reproduction of lattice parameters across multiple phases
- Precise modeling of temperature-dependent octahedral tilting
- Capture of dynamic disorder features observed experimentally

These results validate the LATTE-based model as a reliable, scalable tool for simulating halide perovskites at finite temperatures.
This approach enables deeper exploration of phase stability and local dynamics, which are critical for advancing optoelectronic applications.
Practical Application: Molecular dynamics simulations were used to construct the phase diagram of $CsPbI_3$, which shows improved agreement with experimental data compared to previous studies.

References

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3. W.J. Baldwin *et al.*, *Small* **20**, 2303565 (2023).
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