AI-Assisted Inverse Design of Two-Dimensional Hybrid Perovskites

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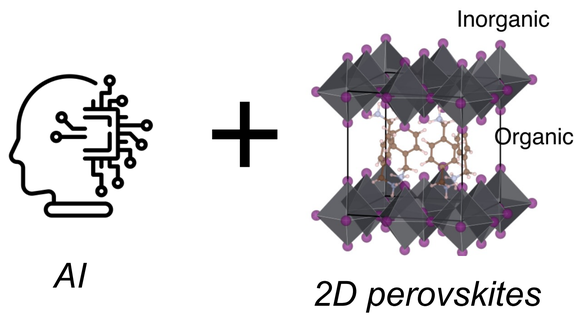
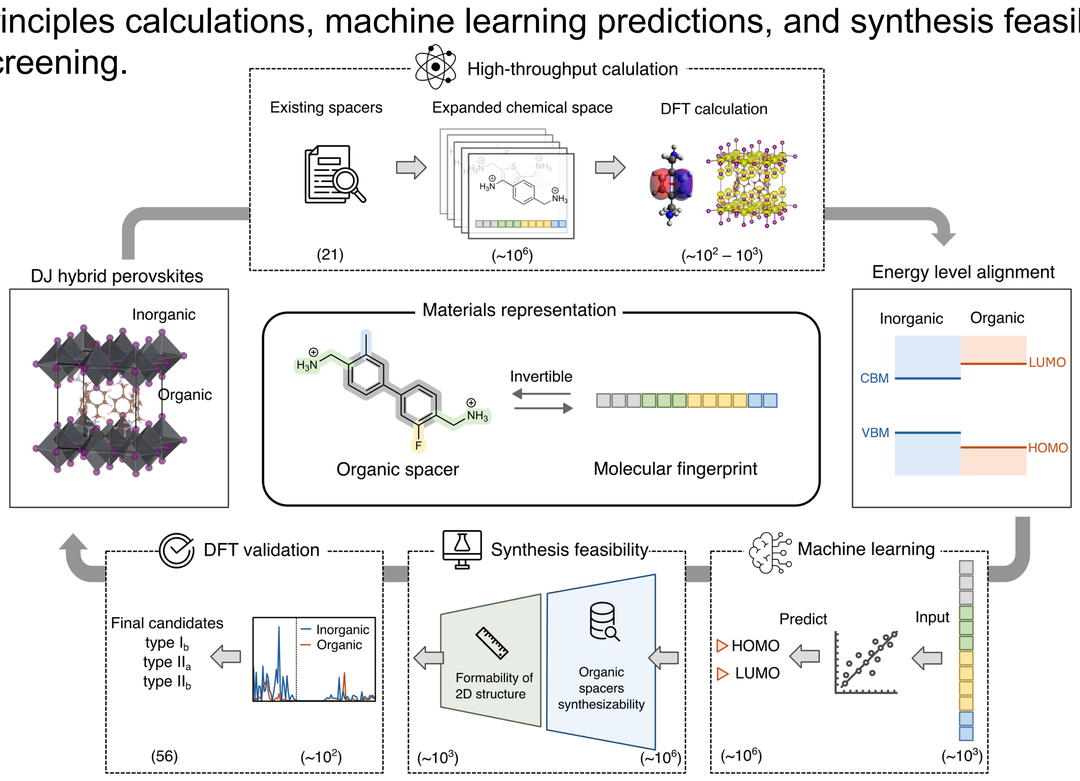


Introduction

- **Artificial intelligence (AI)-assisted workflows** have transformed materials discovery, enabling rapid exploration of chemical spaces of functional material systems.
- Endowed with extraordinary optoelectronic , **two-dimensional (2D) hybrid perovskites** represent an exciting frontier, but current efforts to design 2D perovskites rely heavily on **trial-and-error** and expert intuition approaches, leaving most of the chemical space unexplored and compromising the design of hybrid materials with desired properties.[1]

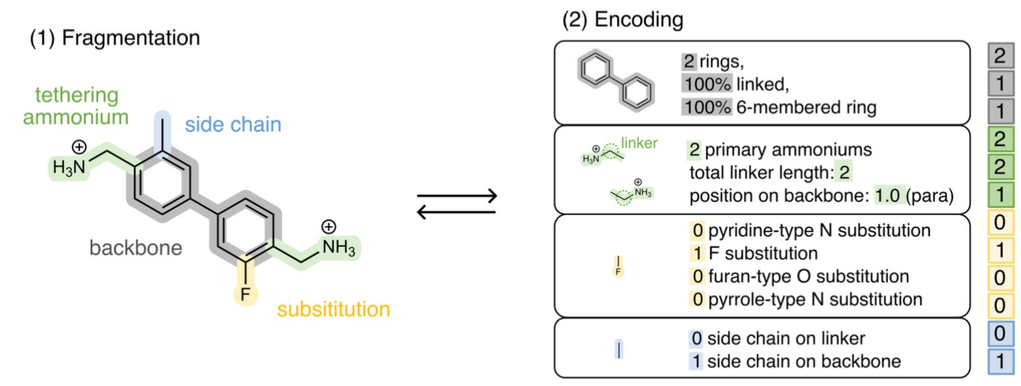
Workflow overview

- We developed an AI-driven workflow that combines high-throughput first-principles calculations, machine learning predictions, and synthesis feasibility screening.



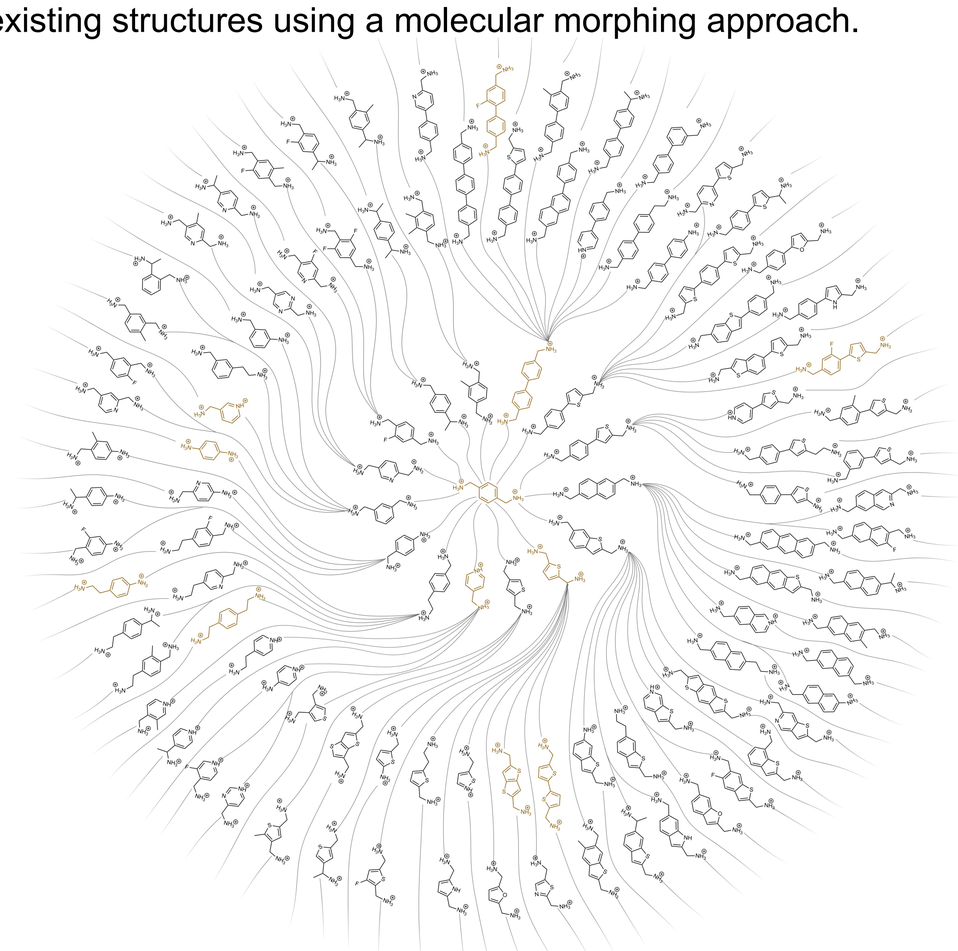
1. Materials representation

- We convert organic molecules into a 12-digit **structural fingerprint**, making the data both machine-readable and interpretable for researchers.



2. High-throughput calculation

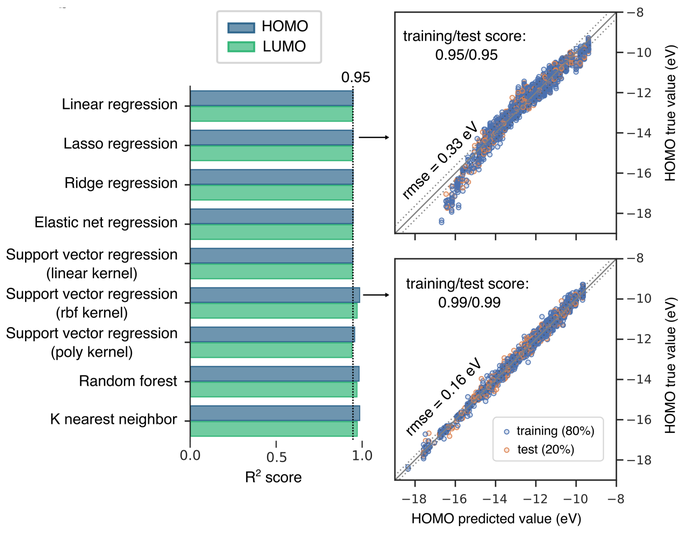
- We generated over ~10^6 hypothetical organic molecules from 21 existing structures using a molecular morphing approach.



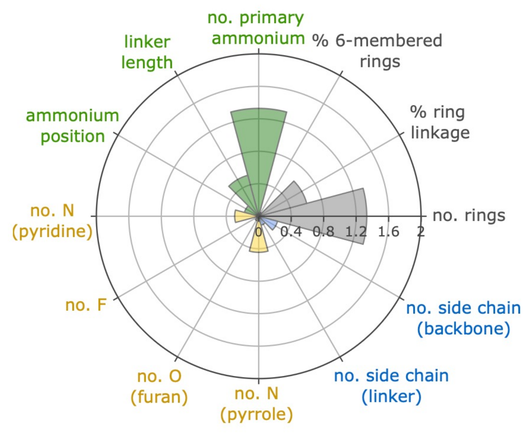
- Using first-principles calculations, we computed the electronic structure of ~10^3 candidates.

3. Machine learning

- Using molecular fingerprint as input features, we trained machine learning models to predict the electronic properties of 2D perovskites.
- These models achieve high predictive accuracy while dramatically reducing the computational cost compared to first-principles calculations.



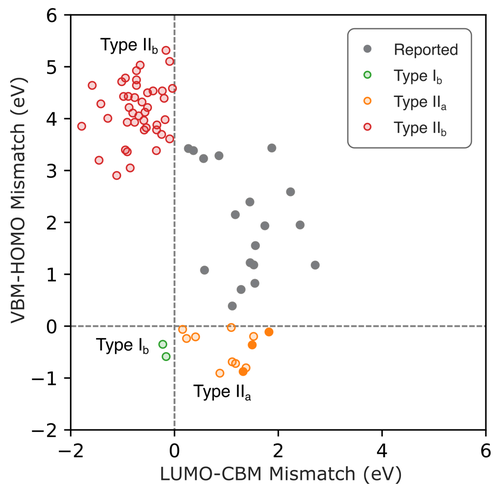
Accuracy of trained models



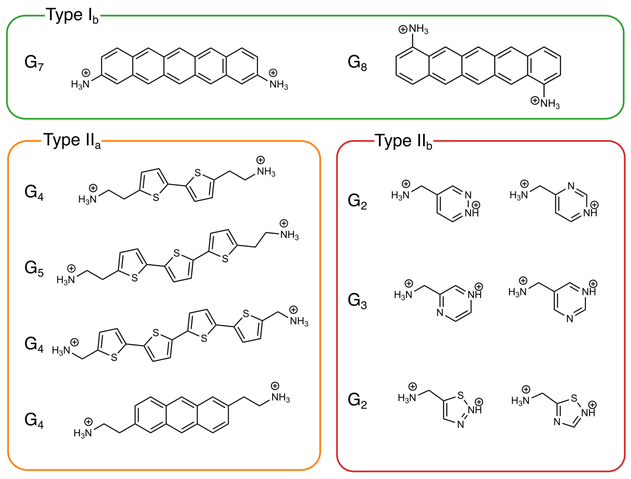
Interpretation of trained models: feature importance

Conclusion and future perspectives

- ✓ We developed an AI-assisted workflow that expands the accessible chemical space of 2D perovskite from 21 initial experimental reported structures to millions of candidate structures.
- ✓ The utility of this workflow is exemplified through the targeted discovery of diammonium organic spacers yielding energy level alignments of type I_b, II_a, and II_b—domains that remain underexplored in the energy landscape of 2D perovskites.
- ✓ This framework is generalizable and can be extended to optimizing alternative properties or applied to other hybrid material systems.



Energetics landscape



Inverse designed candidates

For more information
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References

[1] X. Li, J. M. Hoffman, and M. G. Kanatzidis, The 2D Halide Perovskite Rulebook: How the Spacer Influences Everything from the Structure to Optoelectronic Device Efficiency. Chem. Rev. (2021).