Interpretable Discovery of New Materials

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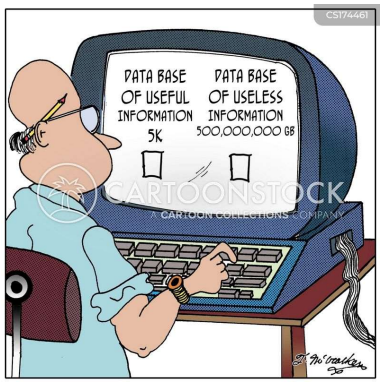
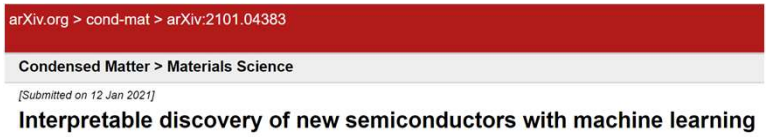


Challenge in accelerated materials discovery

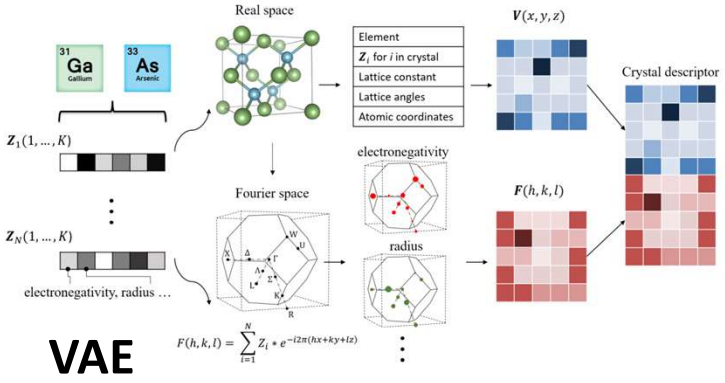
- **Incomplete treasure map of materials discovery**

- **Some of the challenges**:
  - High computational cost of Density Functional Theory (DFT) calculations:
    - Accurate and efficient property prediction
  - Searching the chemical space
    - Brute force search is infeasible
    - Can we do better than random sampling?
  - Generating physical & chemical insights
    - Easy to communicate with experimentalists

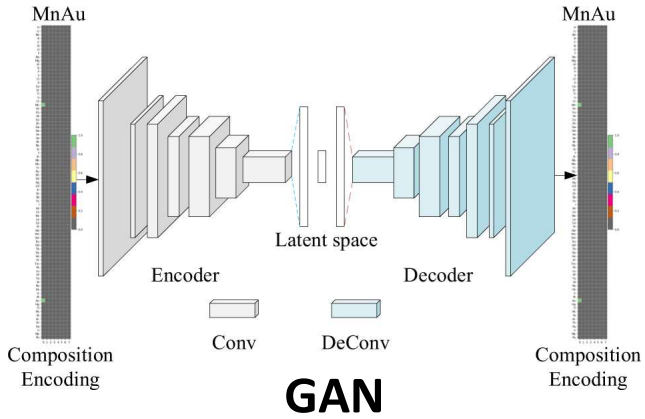
- Can we do all of these without compromising the accuracy?



Some of the existing solutions:



Ref: Inverse design of crystals using generalized invertible crystallographic representation



Ref: Generative adversarial networks (GAN) based efficient sampling of chemical composition space for inverse design of inorganic materials

DARWIN: Deep Adaptive Regressive Weighted Intelligent Network

- Component 1: Surrogate models to predict properties accurately and efficiently
- Component 2: Search algorithms for efficient searching in the discrete space
- Component 3: Unsupervised learning component to distil physics and chemistry from the network

Ref:[2101.04383] Interpretable discovery of new semiconductors with machine learning

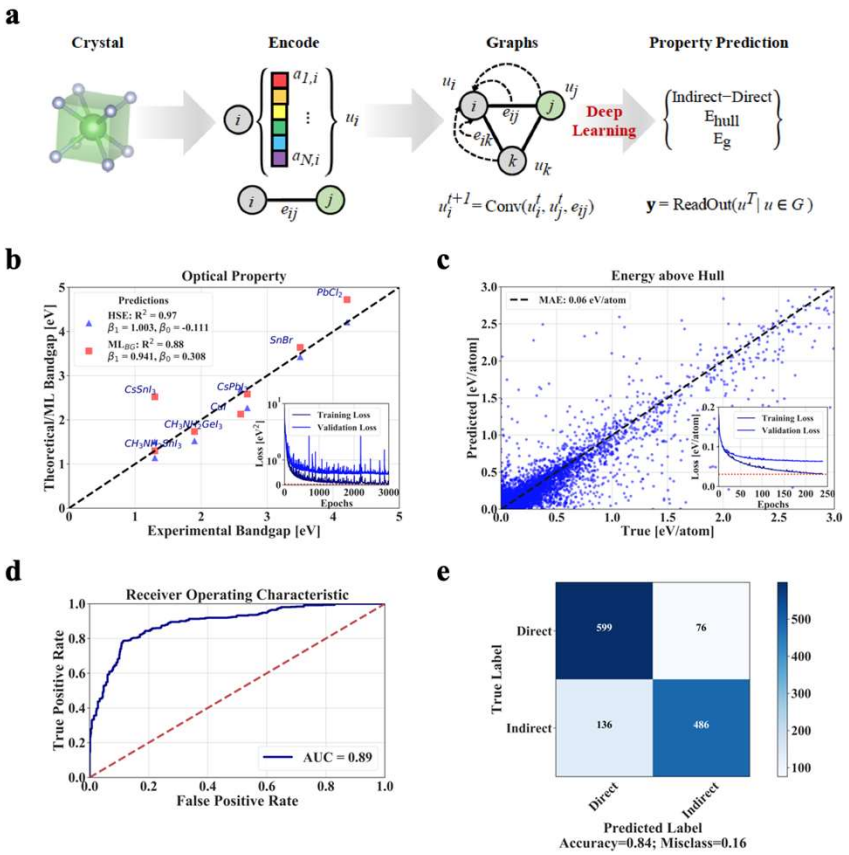
Solution for property prediction

Our target was to find stable (E_{hull} < 0.01 eV/atom), direct bandgap materials with emission just below 400 nm.

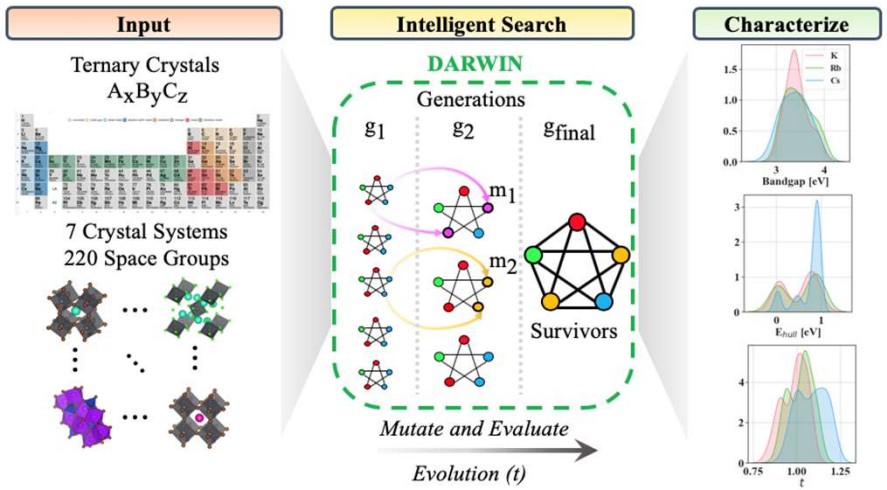
State-of-the-art surrogate models for:

- **Stability using E_{hull}**
- **Bandgap value: HSE06 database**
- **Nature of bandgap (direct vs indirect)**

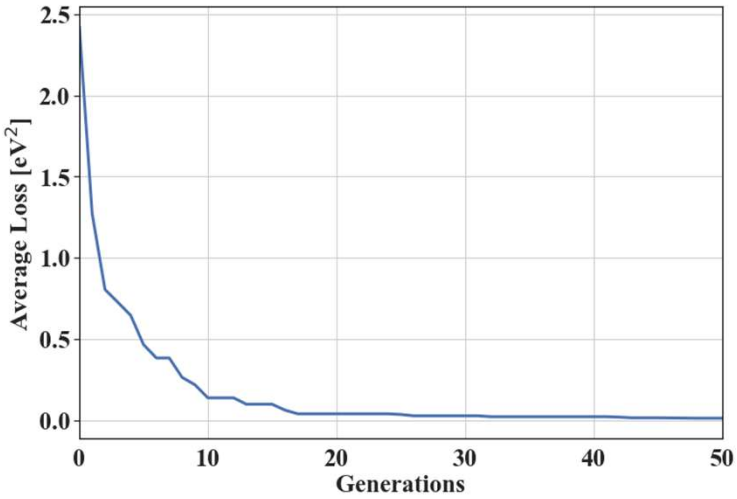
We used convolution operators that incorporated edge weights $\left(\propto \frac{1}{d_{ij}}\right)$



Solution for searching: Genetic Algorithm (GA)



GA exploration with surrogate models



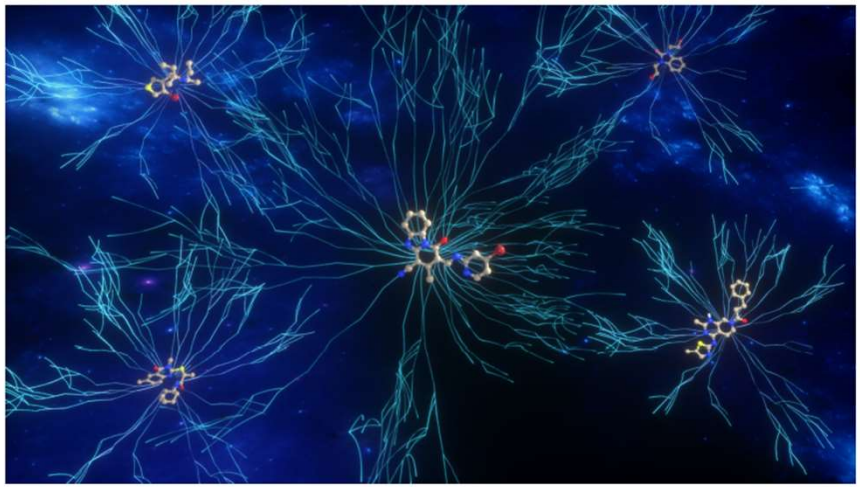
Loss progression with #generations for a stable material with direct bandgap of 3.1 eV

Our target was to find stable (E_{hull} < 0.01 eV/atom), direct bandgap materials with emission just below 400 nm.

Advantage with GA: we get different outcomes for every run.

Do we have any proof of GA's efficiency?

- We do now – 2020 paper by Prof Jan Jensen!
  - Shown for the case of molecules
  - Multiple paths leading to desirable materials



Ref: Henault, E. S., Rasmussen, M. H., & Jensen, J. H. (2020). Chemical space exploration: how genetic algorithms find the needle in the haystack

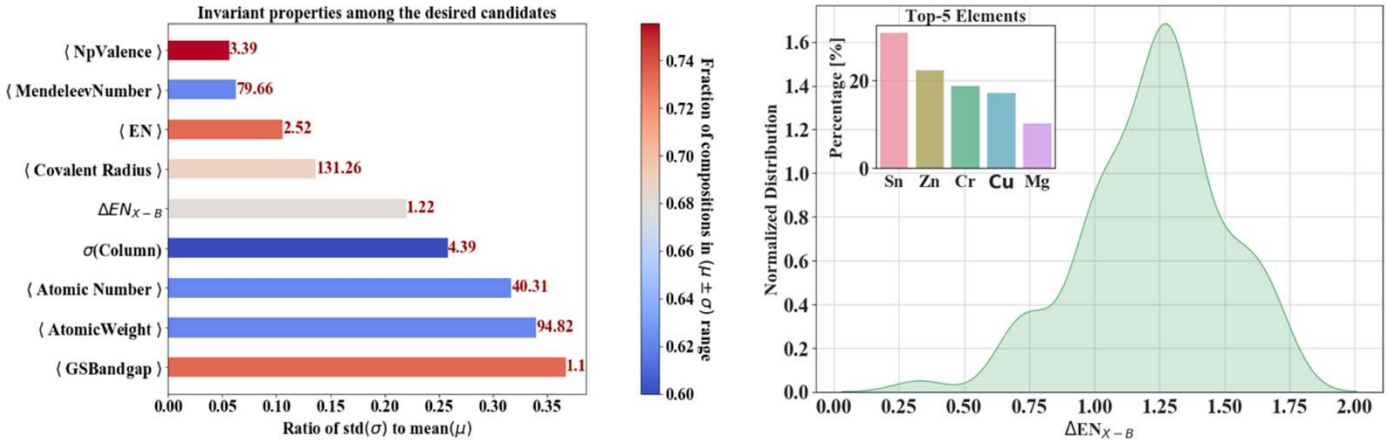
Interpretability:

- ML models: often criticized as black-box
- How can we extract knowledge from accurate machine learning models in a way that can directly be used by experimentalists?
- Several ways of interpretability:
  - Feature importance
  - Analysis of the convolution weights [Lucid by TF team @ tensorflow/**lucid**]
  - Feature imputation (GNNExplainer)

Solution: Unsupervised Learning

- Analyze the output of the GA+ML pipeline using unsupervised learning

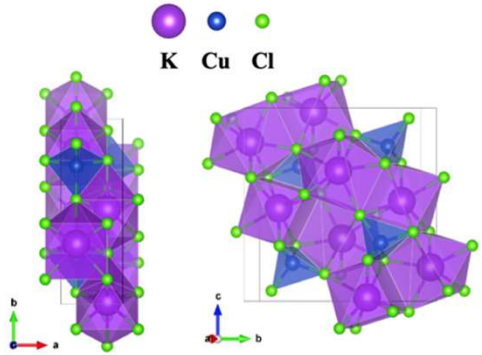
- Ran GA 50 times
  - Collected the candidates
  - Performed frequency analysis on several properties
  - Analysis of properties beyond the ones used in the surrogate models
  - Invariant properties inform us the design rules!

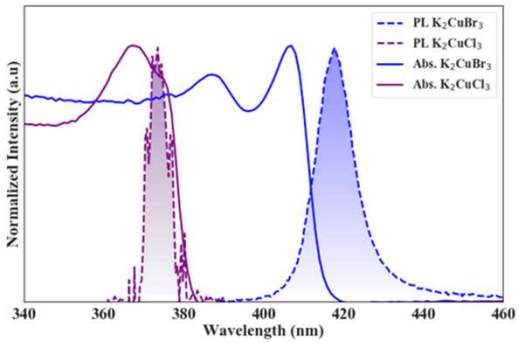


Experimental validation:

- An interesting feature:
  - $\Delta_{X\text{-}B}$ = **(0.95, 1.5): $\mu \pm \sigma$**
  - Electronegativity difference between second most metallic and least metallic element.
  - Optimal Electronegativity Difference Window (OEDW)

- One of the candidates that satisfies this: K_2CuCl_3
  - Met the requirements





Summary:

- GA with surrogate models can be used to efficiently search the chemical space to find materials with desirable properties

- An alternative way to enable interpretability is by performing unsupervised learning on the predicted candidates.
  - Develop new rules-of-thumb that can be used in a lab-setting.

- Replaceable components of DARWIN makes it adaptable!

Thank you!

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