CrysXPP: An Explainable Property Predictor for Crystalline Materials

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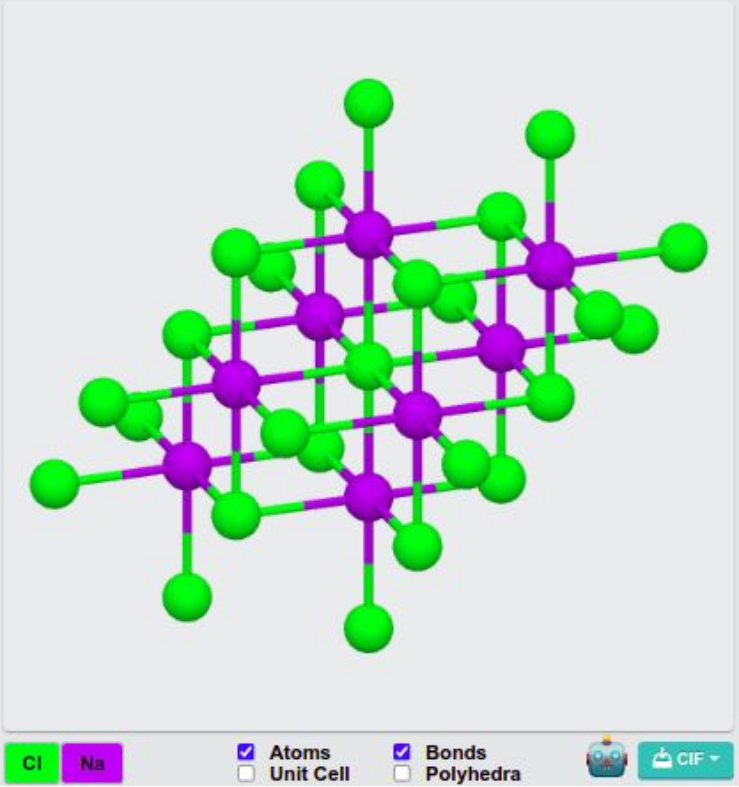
Crystalline Materials

State Properties



Material Details

Final Magnetic Moment
0.000 μ_B

Magnetic Ordering
NM

Formation Energy / Atom
-2.110 eV

Energy Above Hull / Atom
0.000 eV

Density
2.11 g/cm^3

Decomposes To
Stable

Band Gap
5.145 eV

Lattice Parameters

a	4.025 Å	α	60.000°
b	4.025 Å	β	60.000°
c	4.025 Å	γ	60.000°

Volume **46.096 Å^3**

Lattice Structure

Final Structure
Fractional Coordinates

CIF

Na

a	b	c
0	0	0

Cl

a	b	c
0.5	0.5	0.5

Atomic Coordinates

Deep models for crystal property prediction

- **Fast and accurate prediction** of different properties (e.g : State Properties, Elastic Properties etc.) for crystalline materials is a challenging task and has lots of interest to the materials science community since it is **imperative for finding new functional materials**.
- **Density functional theory (DFT)** [Orio et al., 2009] is an effective tool to estimate several chemical Properties, but requires substantial **computation costs.**
- In recent times several **machine learning techniques** [Tian Xie et.al 2018, Chen,C et. al., 2019] have been proposed to enable fast and accurate prediction of different properties for crystalline materials, thus **facilitating rapid screening** over large material search spaces.
- Existing techniques either use **handcrafted feature** based descriptors or deep **graph neural network (GNN)** to generate a representation from the 3d conformation of crystal structures.

Limitation of existing works

- Generating handcrafted features requires specific domain knowledge and human intervention
- Deep models require a huge amount of tagged training data
- DFT error bias in current models.
- Lack of interpretability and algorithmic transparency

Opportunity

- A large corpus of unlabelled crystal data is available, which can be used to learn the structural and chemical information of the atoms and crystal graph in unsupervised way.

Our Proposed Method

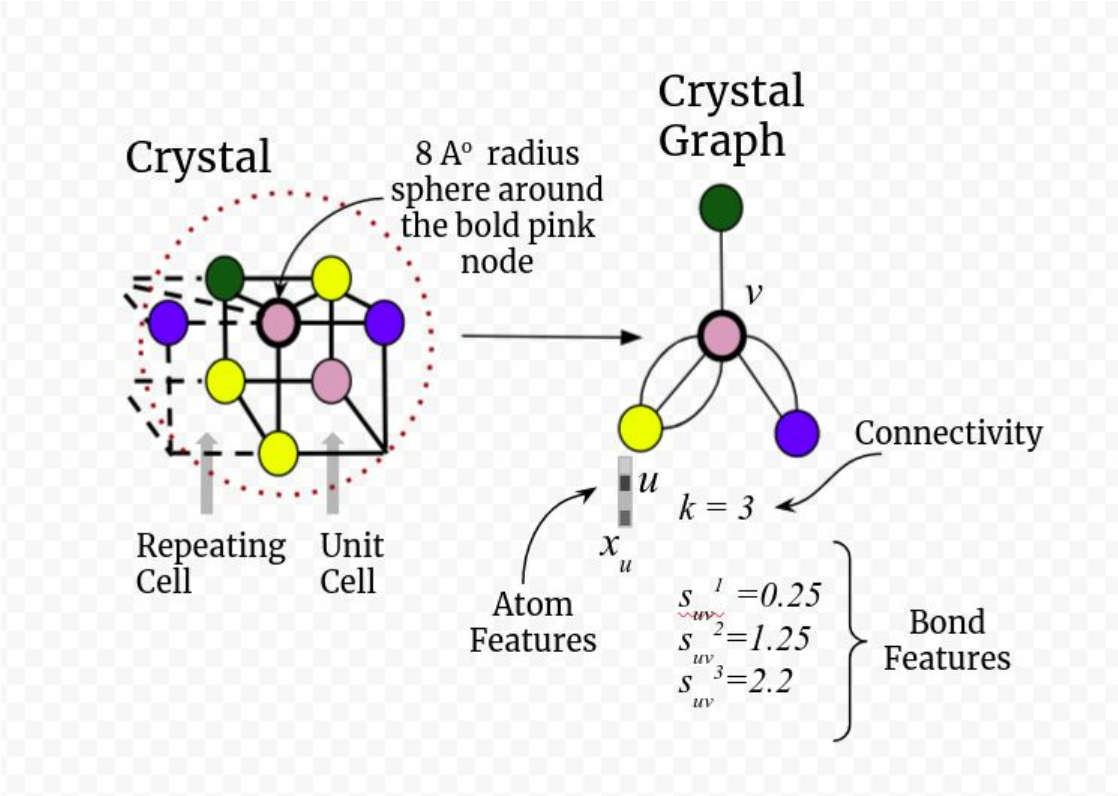
- We propose an explainable deep property predictor for crystalline materials which comprised of two modules :

  CrysAE (**Cry**stal **A**uto **E**ncoder) and **CrysXPP** (**Cry**stal e**X**plainable **P**roperty **P**redictor)

- CrysAE, an auto-encoder based architecture which is trained with a **large amount of unlabeled crystal data** which leads to the deep encoding module **capturing** all the important **structural and chemical information** of the constituent atoms (nodes) of the crystal graph.

- This **learned encoding is leveraged** to build up the property predictor, CrysXPP, to which the knowledge acquired by the encoder is transferred and which is further trained with a **small amount of property-tagged data**, thus largely mitigating the need for having a huge amount of dataset tagged with a specific property.

Graph Representation of Crystal



Atom Features

Features	Range of Values	Dimension
Group Number	1,2, ..., 18	18
Period Number	1,2, ..., 9	9
Electronegativity	0.5–4.0	10
Covalent Radius	25–250	10
Valence Electrons	1, 2, ..., 12	12
First Ionization Energy	1.3–3.3	10
Electron Affinity	-3–3.7	10
Block	s, p, d, f	4
Atomic Volume	1.5–4.3	10

CrysAE (Crystal Auto Encoder)

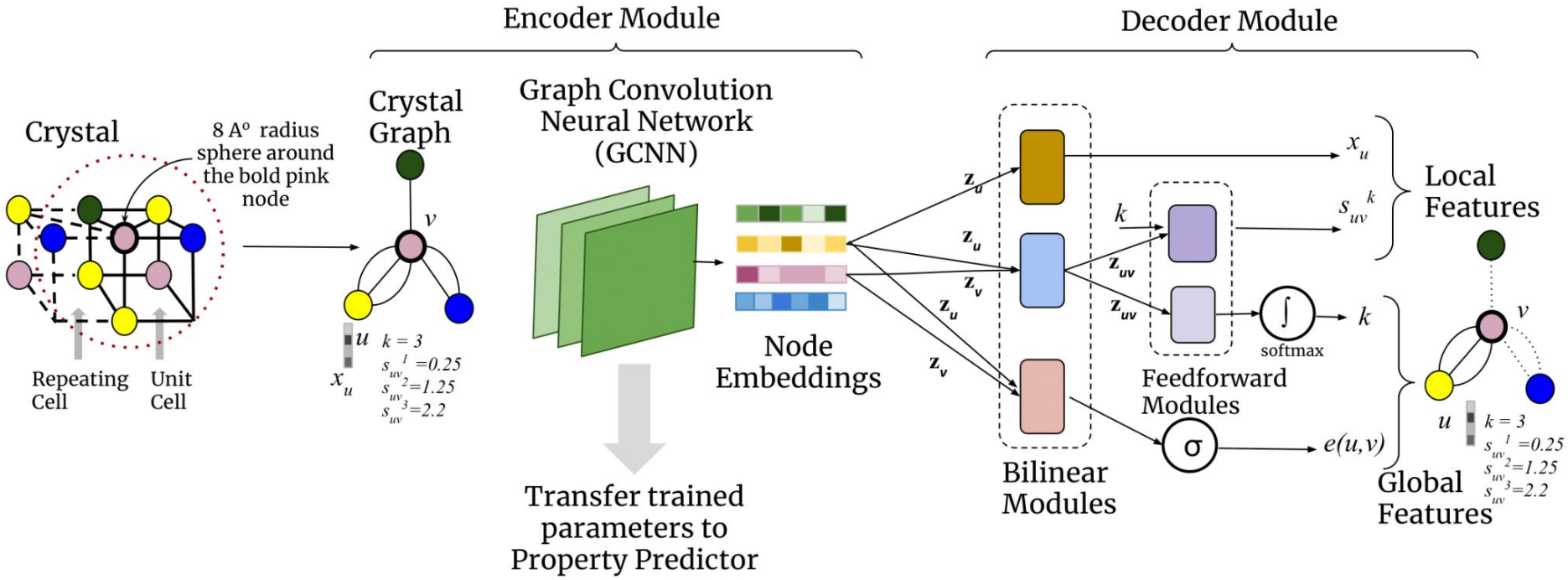
- **Encoder Module :** Crystal graph encoder based on **graph convolution network**, encodes the **chemical and structural information** of a crystal graph into embedding.
- **Decoder Module :** We design an effective decoder which plays an inevitable role in learning the **local and global structure** which are extremely useful. Decoder reconstructs the following :

    i. **Node features**
    ii. **Edge features**
    iii. **Graph Connectivity**

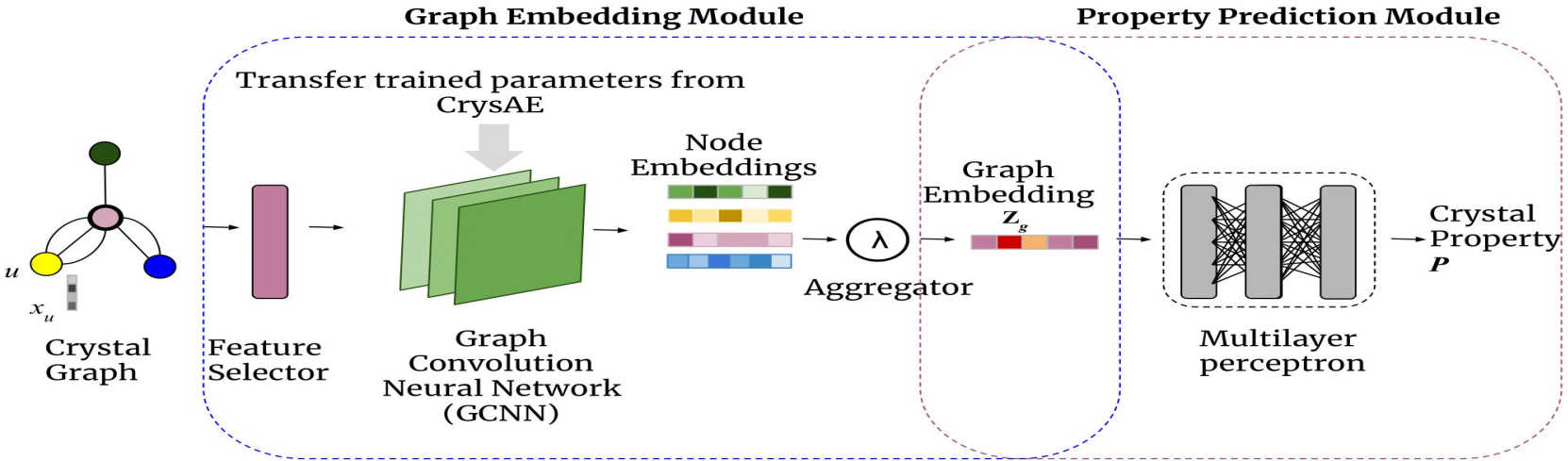
- We learn the trainable parameters of both encoder and decoder end to end by **minimizing these reconstruction loss** of different global and local structural and chemical features.

CrysAE (Crystal Auto Encoder)

Materials Project database
(38000 crystalline materials)

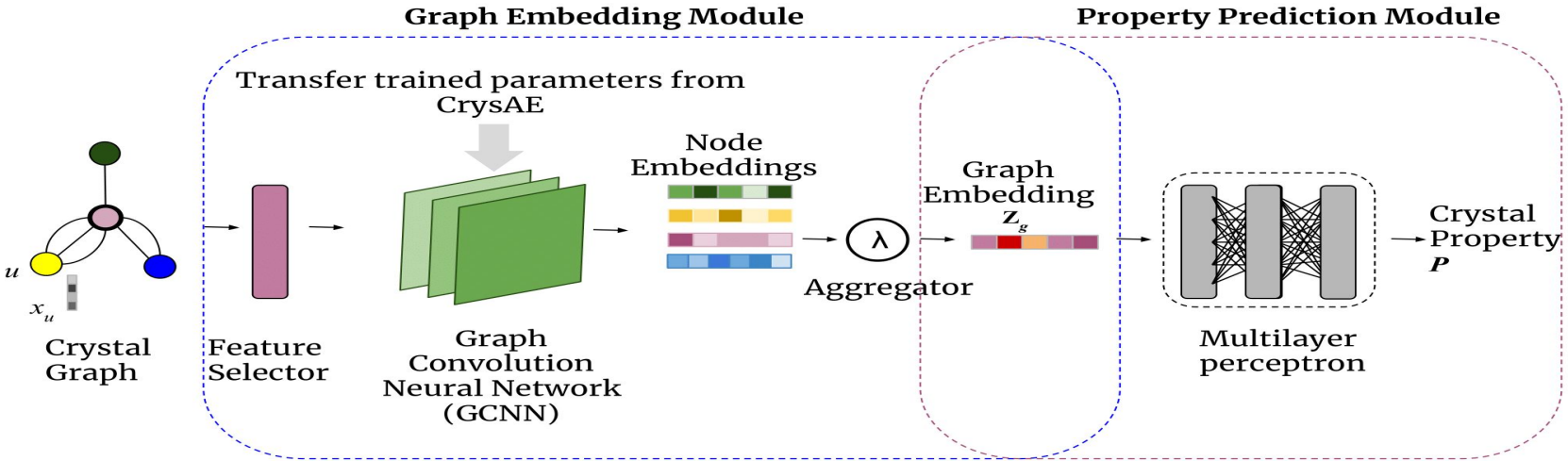


CrysXPP (Crystal eXplainable Property Predictor)



- We build a **model explainability module** by introducing a **feature selector** before the convolution of the node properties.
- The feature selector is a trainable weight vector that **selects a weighted subset of important node level features** for a given property of interest P.
- We use a **LASSO regression** to **impose sparsity** on the feature selector layer.

CrysXPP (Crystal eXplainable Property Predictor)



- Property predictor is designed **specific to a property** that can take the advantage of the structural information learned by the encoder of the CrysAE.
- Use a **symmetric aggregation function** to generate graph embedding from the node embedding (which is invariant of the node orderings).
- Graph Embedding is fed to a **multilayer perceptron** which predicts the value of the properties.

Evaluation

➔ **How effective is the property predictor?**

- How is the the performance of the property predictor especially when it functions with a small amount of DFT tagged data?

➔ **How robust is the structural encoding?**

- Whether the structural encoding helps us to mitigate the noise introduced by DFT calculated properties?

➔ **How effective is the explanation?**

- Cross-validate the obtained explanation with domain experts.

Effectiveness of Property Predictor

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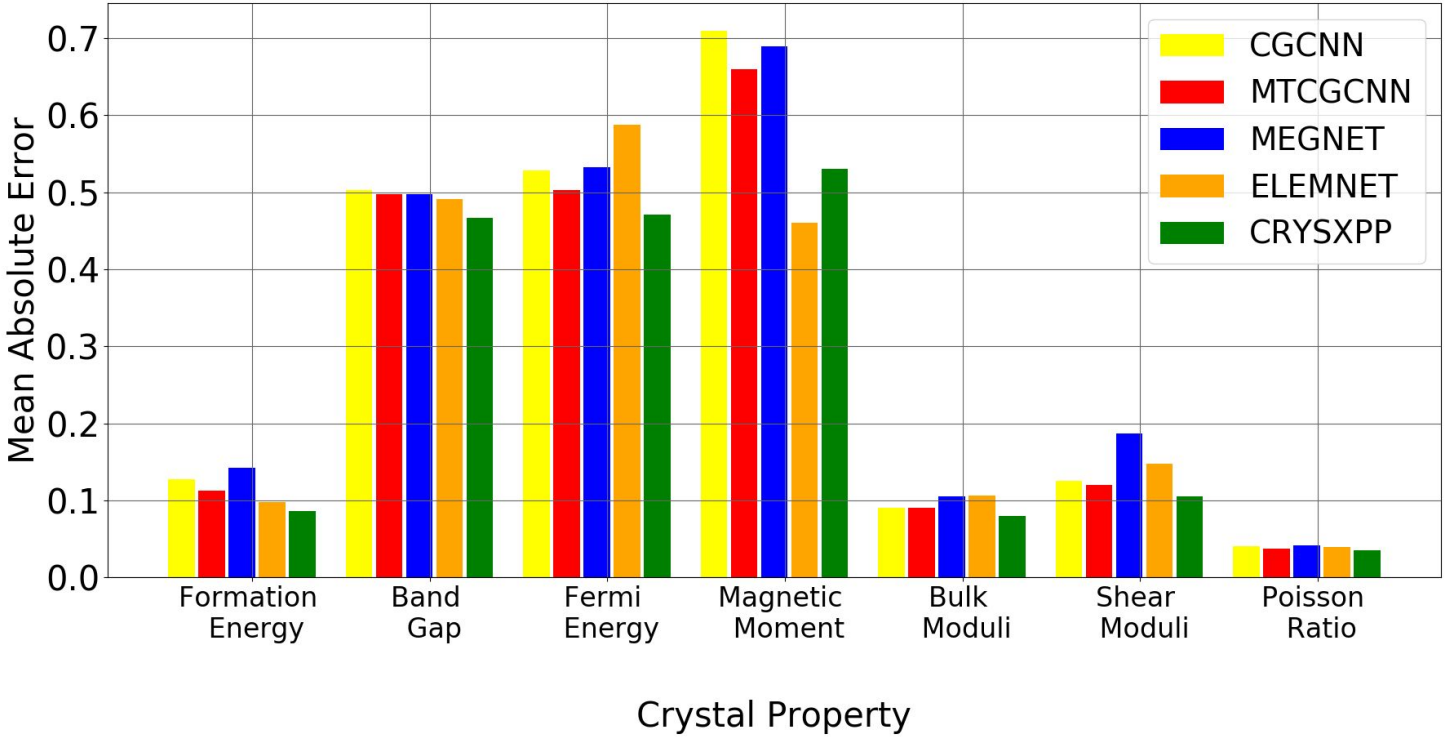


Fig : Summary of the prediction performance (MAE) of different properties trained on 20% data and evaluated on 80% data.

Removal of DFT error bias

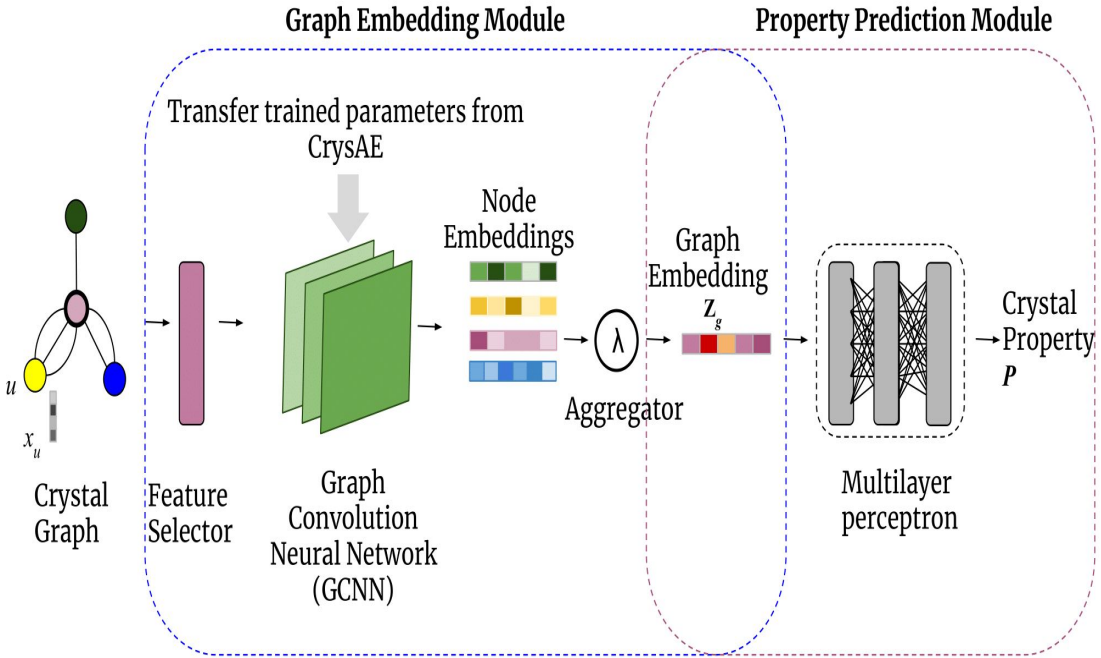
- ➔ **Setup :**
  - We consider a property predictor which has been trained with crystals whose particular property (say Band Gap) values have been theoretically derived using DFT.
  - We then fine tune the parameters with limited amount of experimental data.
- ➔ **Band Gap :** we collect 20 experimental instances from the domain experts, out of which we randomly pick 10 instances to fine-tune the parameters and report the prediction value for the rest

Materials	Exp	DFT	CrysXPP-Exp	CrysXPP
GaSb	0.72	0.36	0.77	0.9
GaP	2.26	1.69	2.10	1.86
GaAs	1.42	0.18	1.54	1.56
InN	1.97	0.47	1.92	1.85
GaN	3.2	1.73	2.11	1.47
NiO	4.3	2.214	2.45	2.08
Si	1.12	0.85	1.08	0.95
ZnO	3.37	1.05	3.42	2.1
FeO	2.4	0	2.25	1.72
MnO	4	0.20	2.31	1.81

TABLE 8: Experiment (Exp) and predicted value for Band Gap for 10 crystals calculated by DFT and other machine learning models after fine-tuned by experimental data.

Explanation through feature selection

- To demonstrate the effectiveness of the feature selector, we present a **case study**



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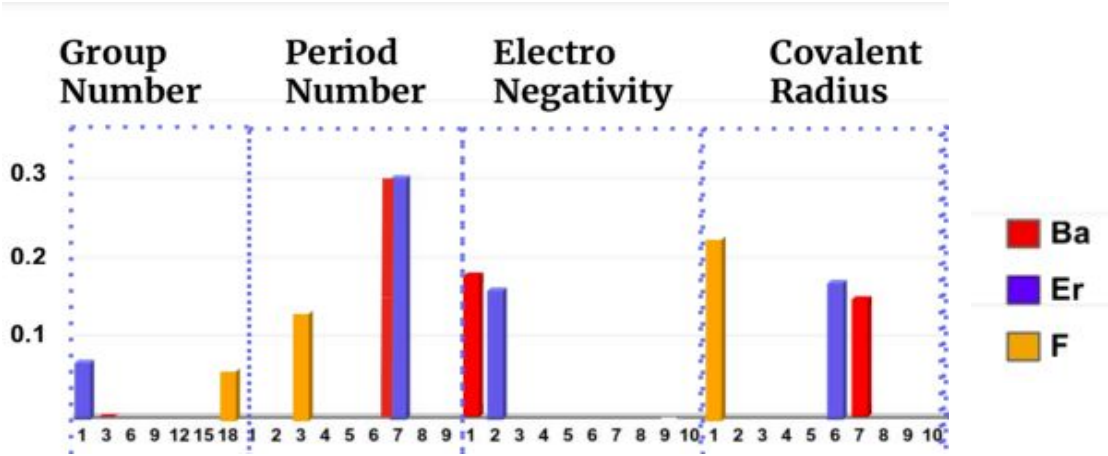
Explanation for Formation Energy



- $BaEr_2F_8$ has Formation Energy -4.41, indicating stability of the materials
- **Period and Group Numbers** provide the information to distinguish each atom.
- Non-zero difference in **Electronegativity** of atoms indicates stability in structure.
- **Covalent Radius** determines the extent of overlap of electron densities of constituents. Higher the radius means weaker the bond. Interesting to note here the trend of weights is the reverse than that of radius itself.

Summary

- In this work, we **propose an explainable property predictor for crystalline materials**, CrysXPP to **predict** different crystal state and elastic **properties with accurate precision using small amount of property-tagged data**.
- We **address the issue of limited crystal data** of a particular property, using transfer learning from an encoding module CrysAE; which we train in a property agnostic way with a large amount of untagged crystal data to capture all the important structural and chemical information useful to a specific property predictor.
- We further find the encoder knowledge is **extremely useful in de-biasing DFT error** using a meagre instances of experimental results.
- With appropriate case studies, we show that the **explanations provided by the feature selection module** are in sync with the domain knowledge.

Thank You for Listening

Any Questions?

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