CrysMMNet: Multimodal Representation for Crystal Property Prediction

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Crystalline Material

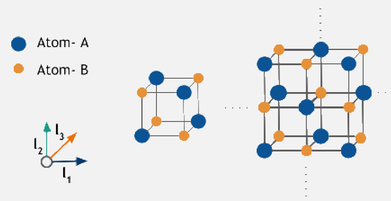


Figure: Structure of Crystalline Materials

- Crystal Material $\mathbf{M = (X, C, L)}$
- Feature Matrix ($\mathbf{X}$): Atomic Feature Set of the Material.
- Coordinate Matrix ($\mathbf{C}$) : Atomic Coordinate Positions.
- Lattice Matrix ($\mathbf{L}$) : describes how a unit cell repeats itself in the 3D space.

- we can represent its infinite periodic structure as

$$\hat{C} = \{\hat{c}_i | \hat{c}_i = c_i + \sum_{j=1}^{3} k_j l_j\}; \ \hat{X} = \{\hat{x}_i | \hat{x}_i = x_i\} \quad (1)$$

where $k_1, k_2, k_3, i \in Z, 1 \leq i \leq n$.

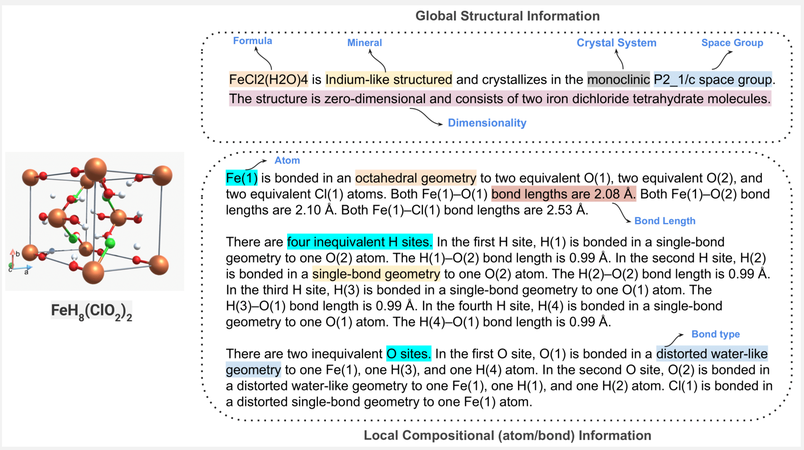
Crystal Property Prediction

- **Task: Given 3D structure of the crystal materials, fast and accurate prediction of different state and electronics properties like formation energy, band gap etc.**
- Existing state-of-the-art models construct multi-edge graphs and apply the GNN model to learn representations of crystal structures that are optimized for downstream property prediction tasks.
- Fail to incorporate crucial global periodic structural information like lattice constraint, space group number, crystal symmetry, rotational information, component 3D orientation, heterostructure information, etc, which will enrich its representation and subsequently aid the property prediction accuracy.

Key Problem: Diverse set of global periodic structural information is difficult to incorporate explicitly into a graph structure.

Our Solution: Learn a more robust and enriched representation by using multi-modal data i.e graph structure and textual description of materials.

Crystal Textual Dataset



$FeH_8(ClO_2)_2$

Figure: Textual description of $\mathbf{FeH_8(ClO_2)_2}$ material from JARVIS dataset generated by Robocrystallographer.

Model Description

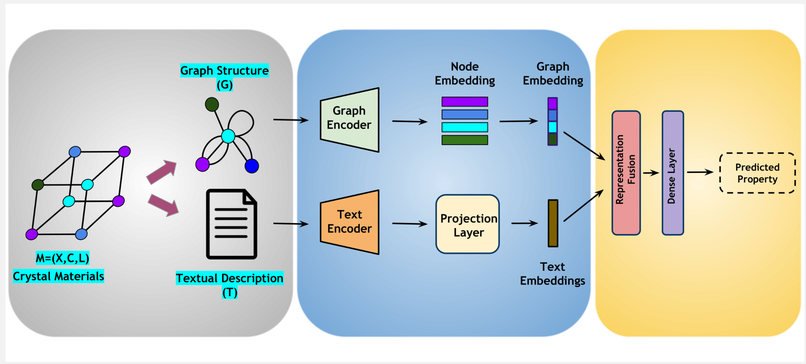


Figure: Overview of our adopted methodology CrysMMNet

Dataset

Curated the textual dataset of two popular materials databases Material Project (MP) and JARVIS forproperty prediction task.

Datasets	Graph Num.	Structural Info.	Textual Info.	Properties	Data Type
MP 2018.6.1	69K	✓	✓	4	DFT Calculated
JARVIS-DFT	55K	✓	✓	6	DFT Calculated

Table: Multi-Modal Datasets Details

Downstream Task Evaluation

Property	CGCNN	SchNet	MEGNET	GATGNN	ALIGNN	Matformer	CrysMMNet
Formation Energy	0.063	0.045	0.047	0.047	0.033	0.033*	**0.028**
Bandgap(OPT)	0.200	0.192	0.145	0.170	0.142	0.137*	**0.128**
Bandgap(MBJ)	0.413	0.433	0.344	0.513	0.310	0.302*	**0.278**
Total Energy	0.078	0.047	0.058	0.056	0.037	0.035*	**0.034**
Bulk Moduli(Kv)	14.47	14.33	15.11	14.32	10.40*	11.21	**9.625**
Shear Moduli(Gv)	11.75	10.67	13.09	12.48	9.481*	10.76	**8.471**

Table: Summary of the prediction performance (MAE) of CrysMMNet for different properties in JARVIS-DFT Dataset.

Robustness of Textual Representation

Property	CGCNN	CrysMMNet (CGCNN)	MEGNET	CrysMMNet (MEGNET)	GATGNN	CrysMMNet (GATGNN)
Formation Energy	0.063	0.046	0.076	0.060	0.077	0.064
Bandgap(OPT)	0.200	0.163	0.184	0.165	0.169	0.157
Bandgap(MBJ)	0.413	0.339	0.369	0.339	0.343	0.331
Total Energy	0.078	0.059	0.058	0.057	0.056	0.053
Bulk Moduli(Kv)	14.47	12.98	15.11	13.29	14.32	13.73
Shear Moduli(Gv)	11.75	10.71	13.09	11.86	12.48	12.04

Table: Summary of the prediction performance (MAE) of different state-of-the-art GNN models with textual representation for six different properties in The JARVIS-DFT Dataset.

Qualitative Analysis Of The Attention Layers

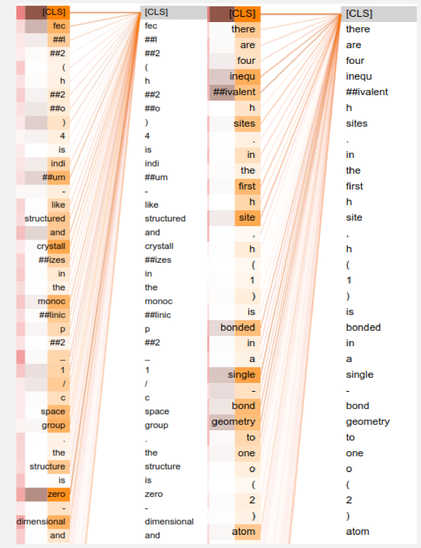


Figure: Attention weights of 5th Layer at MatSciBert between [CLS] token and other tokens in material's description for $\mathbf{FeH_8(ClO_2)_2}$.

Final Takeaways

- Fusing textual representation with graph structure improves crystal property prediction accuracy.
- Textual representation is robust and aid performance improvement in any existing GNN encoder.
- We curated textual datasets of two popular benchmark databases containing both local compositional and global structural information of a material.

References

[1] Xie et. al; **CGCNN**; Phys. Rev. Lett. 2018
[2] Chen et. al; **MEGNET**; Chem. Mater. 2019
[3] Choudhary, et. al; **ALIGNN**; npj Computational Materials 2021
[4] Keqiang Yan et. al; **Matformer**; NIPS 2022

Contact and Paper Information

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Github

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