CRYSTAL GEN:

AI-Driven Crystal Structure Prediction

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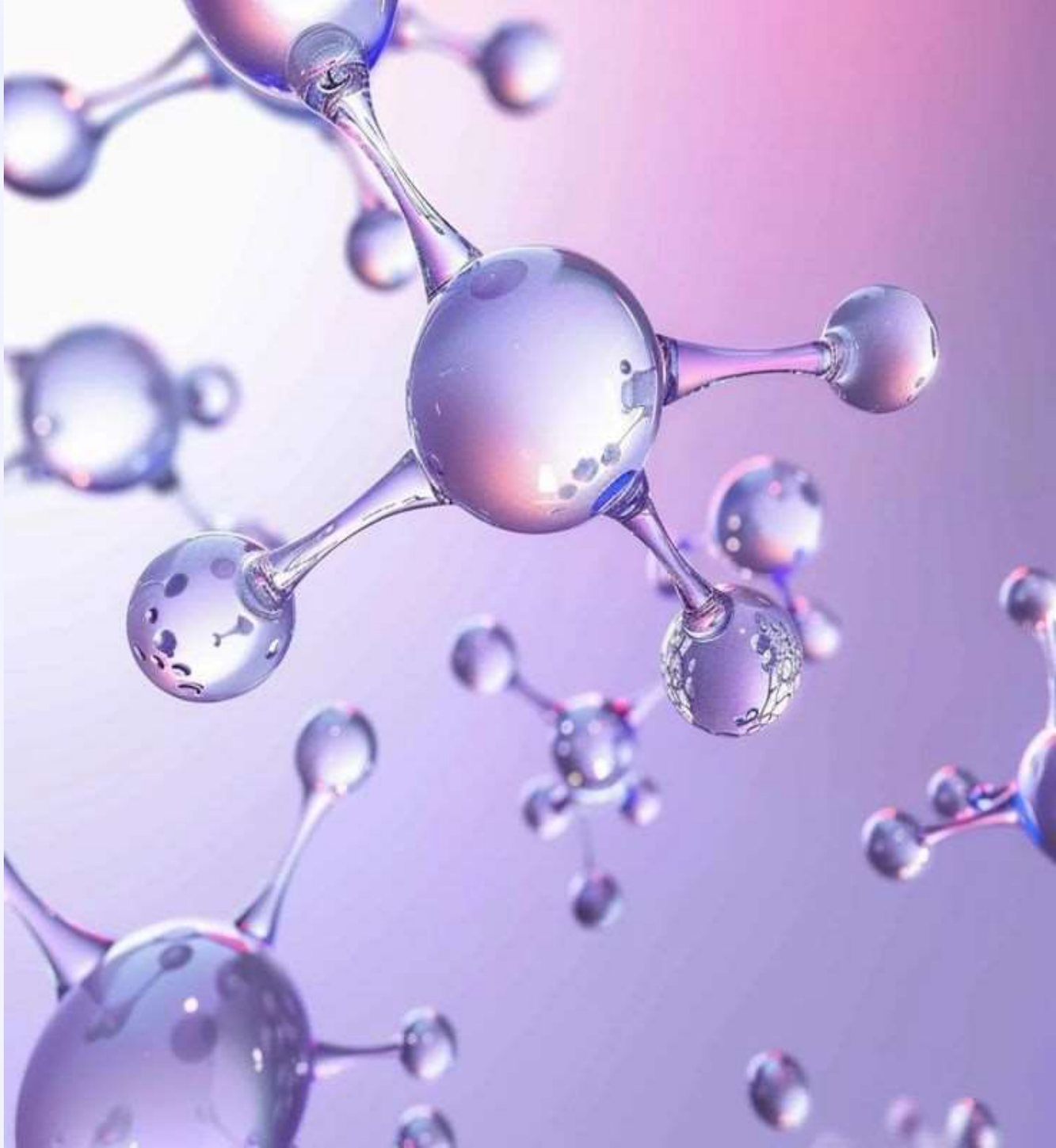
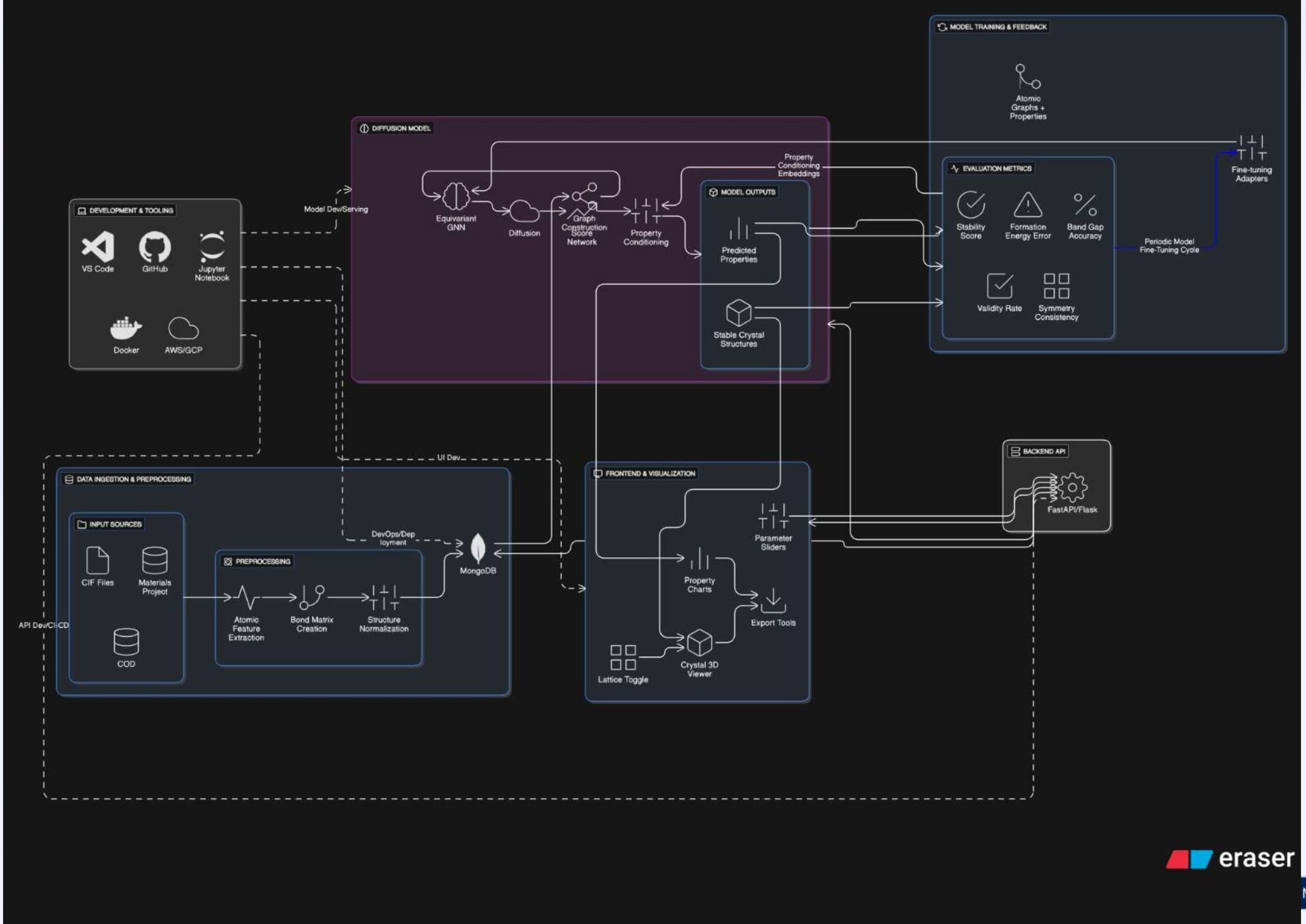
Overview:

CrystalGen is an **AI-powered platform** designed to **predict and analyze crystal structures** from CIF (Crystallographic Information File) data using **Graph Neural Networks (GNNs)**. It **automates the process of crystal analysis**, providing **fast, reliable, and precise insights** into both **structural and chemical properties**. By leveraging advanced machine learning, CrystalGen **significantly reduces manual effort and computational time**, making crystal structure prediction more efficient and accessible.





ARCHITECTURE DIAGRAM:

End-to-End Pipeline Integration
Seamlessly connects data ingestion, model training, diffusion-based generation, and visualization for crystal material discovery.

Data Ingestion & Preprocessing
Ingests crystal structure data from CIF files, Materials Project, and COD; performs atomic feature extraction, bond matrix creation, and normalization stored in MongoDB.

Diffusion Model Core
Combines an **Equivariant Graph Neural Network (GNN)** with a **Diffusion + Property Conditioning Network** to generate stable and property-specific crystal structures.

Model Training & Evaluation
Continuous fine-tuning using metrics such as formation energy error, band gap accuracy, and symmetry consistency; integrates feedback for periodic model improvement.

Frontend & Visualization Layer
Interactive web interface featuring property charts, 3D crystal viewers, and parameter sliders—enabling real-time exploration of generated structures.

Scalable Infrastructure & APIs
Supports **FastAPI/Flask** backend, **Dockerized deployment**, and **cloud (AWS/GCP)** compatibility for scalable serving and development.

Tech Stack:

React

It is a powerful JavaScript library used for building dynamic, component-based user interfaces, enabling efficient rendering and seamless integration with backend APIs.

Flask

It is a lightweight and flexible Python web framework that enables rapid development of APIs and web applications with minimal setup and high customization.

Development Tools

VS code, Github, Jupyter Notebook for development and version control

Diffusion Models

Generative modeling framework enabling iterative denoising to create valid crystals.

MongoDB

It is a No SQL Database used for storing CIF data and generated crystals.

PyTorch

Deep learning framework for building, training, and optimizing the generative model.

Equivariant GNNs

To learn atomic interactions.

Mathematical Foundation:

Reparameterization:

Allows the model to sample a latent variable z from a distribution while keeping the process differentiable.

$$z = \mu + \sigma \odot \epsilon, \quad \epsilon \sim \mathcal{N}(0, I)$$

KL Divergence:

Measures how much the learned latent distribution $q(z \mid x)$deviates from the prior $p(z)$)usually $\mathcal{N}(0, I)$)
Encourages the latent space to stay close to a standard normal distribution:

$$\mathcal{L}_{KL} = -\frac{1}{2}\sum(1 + \log\sigma^2 - \mu^2 - \sigma^2)$$

Total Losses:

Combines **reconstruction loss** (data fidelity) and **KL divergence** (regularization).
Ensures balance between accurate reconstruction and smooth latent space

$$\mathcal{L} = \mathcal{L}_{lattice} + \mathcal{L}_{frac} + \mathcal{L}_{species} + 10^{-3}\mathcal{L}_{KL}$$

Reconstruction Losses:

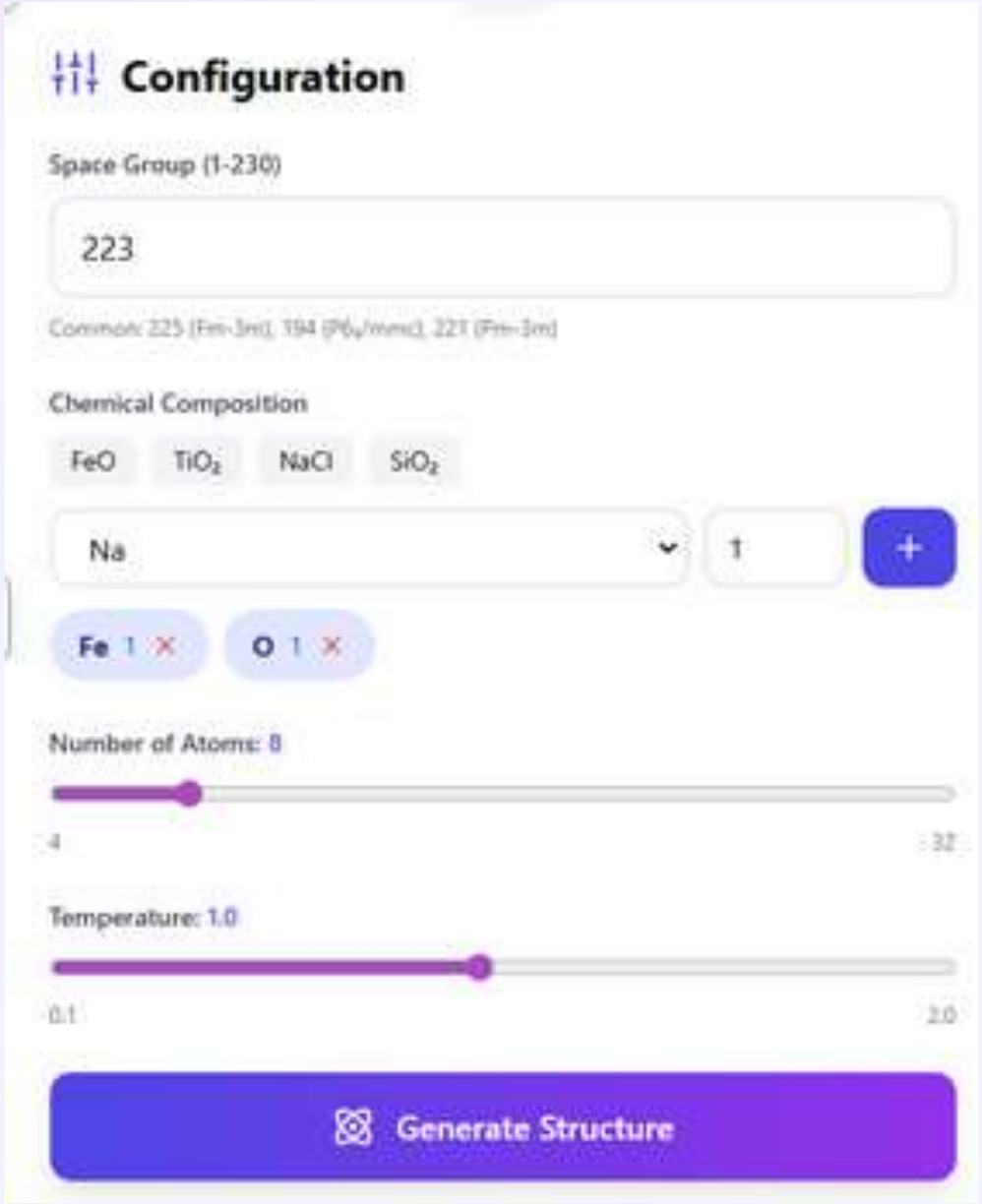
Measures how well the decoder reconstructs the input structure (lattice, fractional coords, species).
Typically includes MSE for continuous outputs and Cross-Entropy for categorical outputs:

Sampling:

Generates new crystal structures by decoding random late

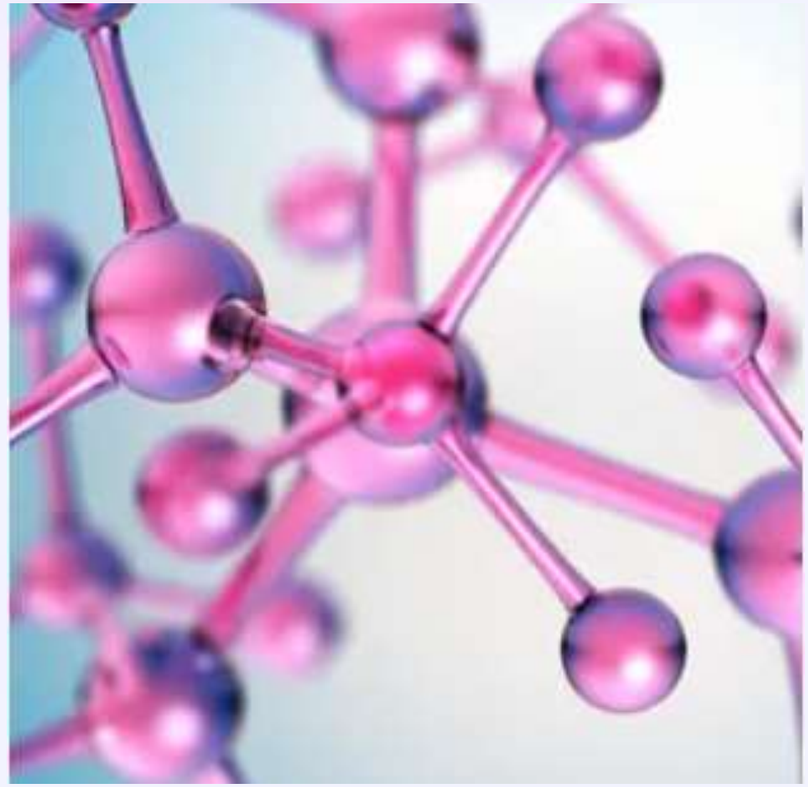
$$z \sim \mathcal{N}(0, I); \quad (\hat{L}, \hat{F}, \hat{S}) = \text{Decoder}(z)$$

IMPLEMENTATION:



IMPROVEMENTS:

Enhanced the existing architecture by integrating **Graph Neural Networks (GNNs)** for learning atomic-level interactions and improving crystal property prediction. Developed a complete workflow with **CIF data preprocessing**, a **Flask–React web interface**, and **interactive 3D crystal visualization** for intuitive exploration and analysis.



Explored how **graph-based deep learning** effectively models atomic connectivity and spatial symmetry. Gained practical understanding of **latent space representation**, model fine-tuning, and performance optimization. Future improvements include integrating **Diffusion or Transformer-based models** for greater generative accuracy, implementing **stability verification**, and extending the dataset with **complex multi-component materials**.

Real-World Applications

Applicable to **crystal and material discovery**, **drug molecule design**, **semiconductor research**, and **energy storage materials**, enabling faster and more accurate innovation in materials science.

OUR WORK:

1

Performance Analysis

•The GNN-based model demonstrated improved accuracy in predicting **formation energy** and **stability** compared to baseline architectures.
•Integration of **conditional latent variables** enhanced structure-property correlations.
•**3D visualization and CIF preprocessing** significantly reduced manual effort in structure validation.
•The model achieved consistent **reconstruction quality** across diverse material types.

2

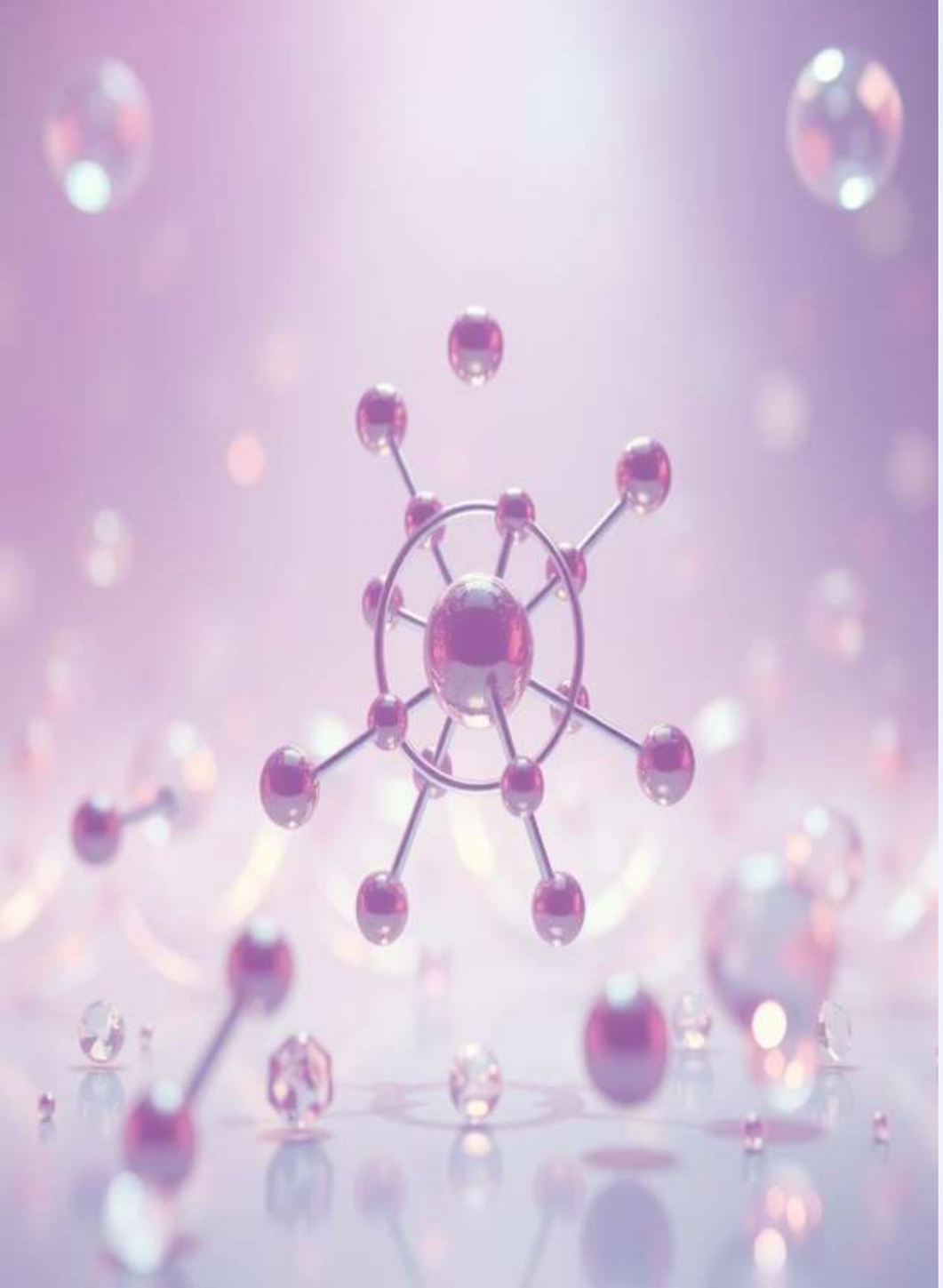
Challenges Faced

•Handling **large and irregular crystal graphs** led to higher computational demands.
•**CIF parsing and data standardization** required extensive preprocessing due to inconsistent formats.
•Ensuring **stability and physical validity** of generated structures remained a non-trivial task.
•Hyperparameter tuning and achieving convergence in **CVAE–GNN hybrid models** were time-intensive.

3

Limitations

•The current dataset is limited to **simple or small-unit cell materials**, affecting generalization to complex crystals.
•Lack of **experimental validation** restricts real-world reliability.
•**Diffusion-based or Transformer architectures** not yet implemented, limiting generation diversity.
•**Stability scoring** and property prediction need further refinement for production-level deployment



CONCLUSION:

CrystalGen showcases the power of AI and Graph Neural Networks in accelerating crystal structure prediction and generation, enabling rapid, data-driven material discovery with interactive 3D visualization.

THANK YOU!