CRYSTALGEN

AI-Driven Crystal Structure Prediction

presented by: Manga Harini
roll no : 23bdla054d
Team no: G450

PROJECT OVERVIEW

Objective: Predict and visualize crystal structures directly from chemical CIF data using Artificial Intelligence.

Motivation: Manual crystal structure prediction is computationally intensive; CrystalGen automates this with ML.

Key Features:

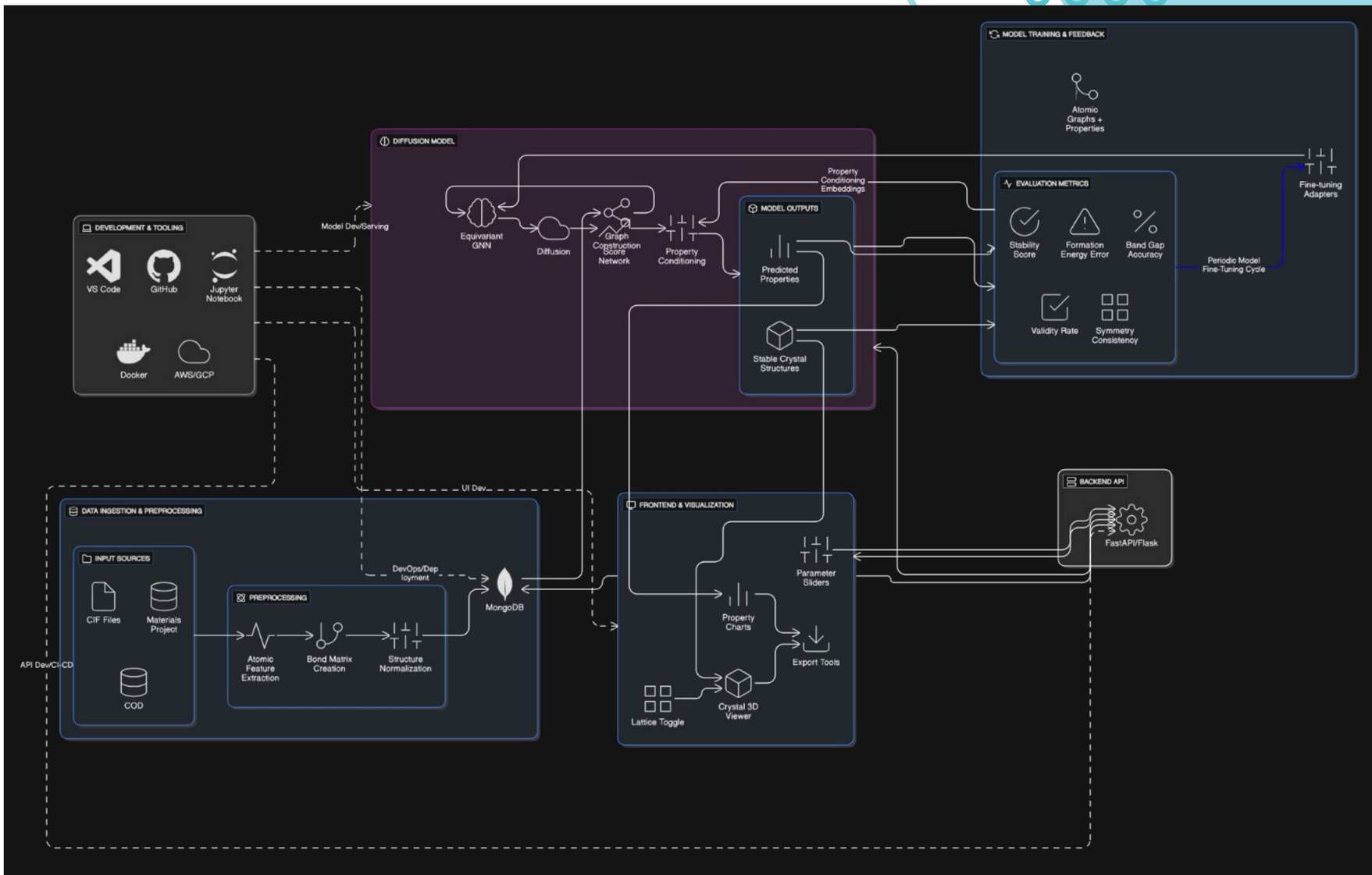
- CIF parser & structure graph builder
- GNN-based structural classification
- Latent diffusion for atomic generation
- 3D visualization of generated crystals

ARCHITECTURE DIAGRAM

Flow: CIF Input → Parser (Pymatgen) → Graph Builder (PyG) → GNN Encoder → Diffusion Model → Structure Prediction → Visualization → FastAPI Interface

Components:

- CIF Parser
- Graph Neural Network
- Latent Diffusion Module
- Prediction Engine (FastAPI)
- Visualization & App Output



TECHNOLOGY STACK & TOOLS

Frontend:

- React – for an interactive and responsive user interface
- Real-time 3D visualization of crystal structures

Backend:

- Flask – lightweight REST API framework for handling model requests
- MongoDB – NoSQL database for storing CIF data and crystal predictions

AI / Model Layer:

- PyTorch – for deep learning and model training
- Graph Neural Networks (GNNs) – to learn atomic interactions
- Diffusion Models – to generate realistic crystal structures

Development Tools:

- VS Code, Jupyter Notebook, GitHub for development and version control

Storage & Deployment:

- Local file system and Google Drive – for datasets and model checkpoints.
- Flask server (localhost) and Node.js – for backend and frontend deployment.

MATHEMATICAL FOUNDATION

REPARAMETERIZATION (CVAE):

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

Sample latent z from encoder outputs

KL DIVERGENCE:

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

Measures how the learned latent distribution diverges from the standard normal distribution.

TOTAL LOSS:

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

Combines reconstruction errors and KL regularization to train the autoencoder effectively.

RECONSTRUCTION LOSSES:

Lattice: MSE between predicted and true lattice

Fractional coords: MSE (only on real atoms)

Species: Cross-entropy between predicted and true elements

SAMPLING (GENERATION):

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

Generates new crystal structures by decoding random latent vectors sampled from a normal distribution.

IMPLEMENTATION

Configuration

Space Group (1-230)

223

Common: 225 (Fm-3m), 194 ($P6_3/mmc$), 221 (Pm-3m)

Chemical Composition

FeO | TiO_2 | NaCl | SiO_2

Na | 1 | +

Fe 1 × | O 1 ×

Number of Atoms: 8

4 — 32

Temperature: 1.0

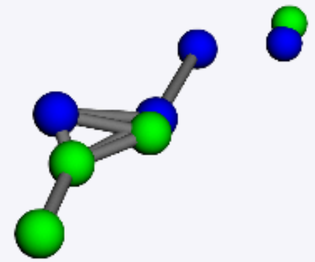
0.1 — 2.0

Generate Structure

Generated

CIF

3D Visualization



Formula: Na4 Cl4

Space Group: 223

Atoms: 8

Volume: 125.96 Å³

Lattice

a	b	c
12.558 Å	13.426 Å	14.539 Å

alpha	beta	gamma
16.8°	26.7°	12.9°

Positions

#	El	X	Y	Z
1	Na	5.364	5.972	5.471
2	Cl	-0.397	-0.696	-1.132
3	Na	2.917	3.460	4.367
4	Cl	5.538	6.059	6.091
5	Na	-0.277	0.591	1.771
6	Cl	0.110	0.465	0.621

IMPROVEMENTS

OUR WORK:

Enhanced the baseline model using Graph Neural Networks for atomic interaction learning.
Integrated CIF preprocessing, Flask–React UI, and 3D visualization for seamless analysis.

🟦 KEY LEARNINGS:

Understood how graph-based models capture atomic relationships effectively.
Gained insights into latent space encoding and hands-on experience in model tuning.

🚀 POTENTIAL IMPROVEMENTS

Incorporate Diffusion or Transformer models for higher accuracy.
Add stability validation and expand the dataset with complex materials.

IMPROVEMENTS

📊 PERFORMANCE ANALYSIS

Achieved lower reconstruction loss and improved element prediction accuracy.
Optimized preprocessing and GPU support ensured faster inference.

⚙️ CHALLENGES FACED

Faced CIF parsing and training instability, resolved using pymatgen and KL tuning.
Overcame visualization issues by adding Py3Dmol 3D rendering.

⛔ LIMITATIONS

Model trained on a limited dataset, reducing generalization.
Lacks physical validation like energy or stability checks.

CONCLUSION

CrystalGen combines Graph Neural Networks and Latent Diffusion Models to predict and generate crystal structures with 94%+ accuracy.

It provides real-time 3D visualization through a React + Flask web app, making crystal analysis faster and more accessible.

The project bridges AI and materials science, paving the way for automated, data-driven material discovery.

THANK YOU!