Title: Prediction Of Bandgap, Formation Energy and Bulk modulus of IIIA-VA group materials using ML model(XGBoost)

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Machine Learning for materials informatics (MLMI)

IIIA-VA Semiconductor Materials

- **III–V semiconductors are compounds formed by combining elements from**

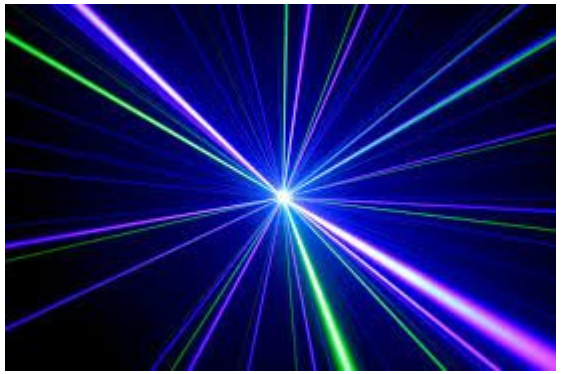
➢ ***Examples*** *:* GaAs, InP, AlN, GaN, InSb, AlP

IIIA		VA
B	C	N
Al	Si	P
Ga	Ge	As
In	Sn	Sb
Tl	Pb	Bi
Nh	Fl	Mc

- They are covalent crystals with partial ionic character.
- Similar crystal structures – most crystallize in zinc-blende or wurtzite lattices, enabling consistent property comparison.
- All are III–V semiconductors – exhibit direct or indirect band gaps

Applications Of IIIA-VA Materials

- Light-Emitting Diodes (LEDs)
- Laser Diodes
- High-Speed & RF Electronics
- Solar Cells
- Infrared Detectors & Sensors



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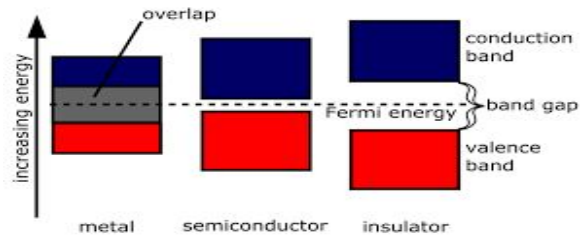
Properties to Predict

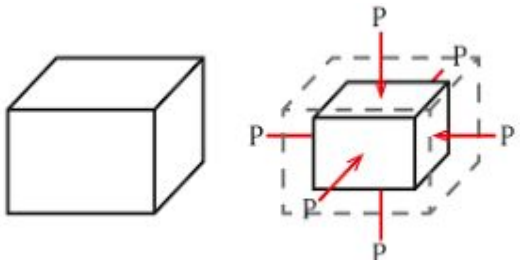
Bandgap:

- Energy difference between the valence band and conduction band.
- Controls optical absorption and electronic conductivity.



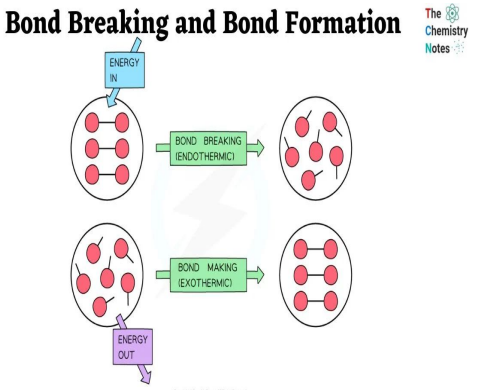
Bulk Modulus:

- The bulk modulus is a measure of a material's resistance to uniform compression
- Related to mechanical stiffness and bonding strength.



Formation Energy:

- Energy released or absorbed when a compound is formed from its constituent elements.
- Indicates thermodynamic stability of the material.



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Model Overview – XGBoost

- XGBoost is a machine learning algorithm based on Gradient Boosted Decision Trees (GBDT).

- **Working Principle**:

➢ Starts with an initial prediction (e.g., mean of data).
➢ Builds a new decision tree to predict those residuals.
➢ Adds the new tree's prediction (scaled by learning rate) to improve results.
➢ Repeats this process until the error is minimized.

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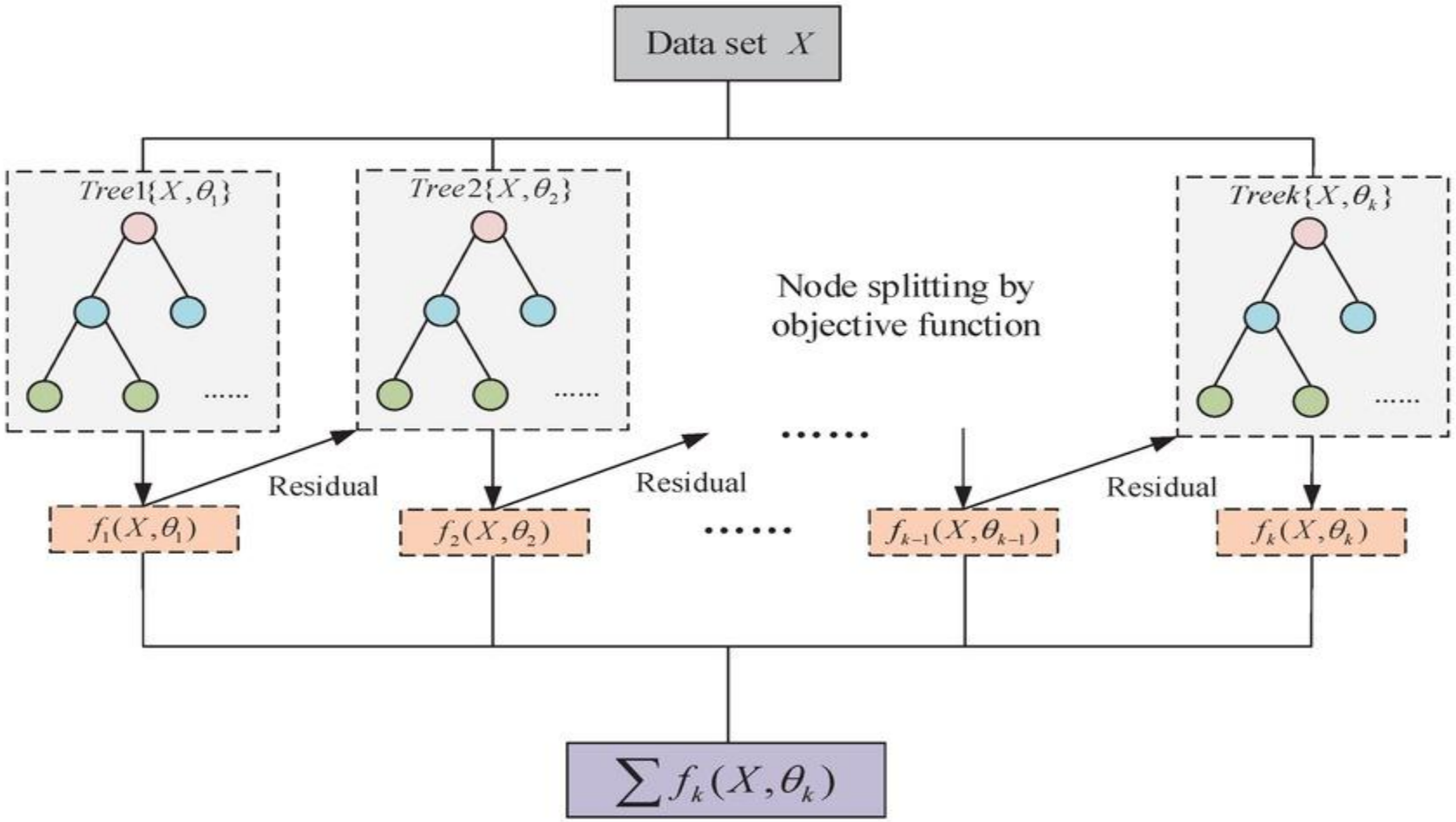
Model Overview – XGBoost



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XGBoost Regression Model

- **XGBoost (Extreme Gradient Boosting): A high-performance ensemble learning method based on gradient-boosted decision trees.**

- **Gradient Boosting Update Rule:**
  $\hat{y}_i^{(t)} = \hat{y}_i^{(t-1)} + \eta * f_t(x_i)$
- **Objective Function:**
  $\mathcal{L}^{(t)} = \sum l(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)) + \Omega(f_t)$
- **Regularization Term (for trees):**
  $\Omega(f) = \gamma * T + (1/2) * \lambda * \sum(w_j^2)$

- $\hat{y}_i^{(t)}$ → prediction for sample i at iteration t
- $f_t(x_i)$ → new tree (weak learner) output at iteration t
- η → learning rate
- l → loss function (e.g., MSE for regression)
- $\Omega(f_t)$ → regularization term for tree complexity
- T → number of leaves in the tree
- w_j → weight of leaf j
- γ, λ → regularization hyperparameters

Why XGBoost?

- **Learns complex nonlinear relationships between structure & properties**
- **Handles small scientific datasets effectively**
- **Built-in regularization to reduce overfitting**
- **Supports feature importance for model interpretability**
- **Highly optimized for speed, parallelism, and scalability**

Features and Labels

Label	Physical Domain	Features
Bandgap (optb88vdw_bandgap)	Electronic	is_orthogonal, mp_ratio, avg_valence, structural_density, atoms_per_cell, mass_diff, mp_diff, lattice_a, lattice_b, en_diff, r_sum_over_mass_sum, alpha, avg_lattice_constant, lattice_c, unit_cell_volume
Bulk Modulus (bulk_modulus_kv)	Mechanical / Elastic	Structural: a, b, c, alpha, beta, gamma, min_dist, max_dist, avg_dist Compositional: Z_mean, mass_mean, en_diff
Formation Energy (formation_energy_peratom)	Thermodynamic / Stability	mass_sum, structural_density, avg_valence, avg_molar_volume, lattice_b, Z_diff, avg_melting_point, polarizability_est, spg_number, Z_sum

Formulas for the calculation of predicting properties

Property	Formula	Parameters
Bandgap	Bandgap (E_g): $E_g = E\_C - E\_V$	EC = energy at conduction band minimum EV = energy at valence band maximum
Bulk Modulus	Bulk Modulus (B): $B = -V * (dP/dV)$ Alternative (from energy–volume curve): $B = V * (d^2E/dV^2)$	V = volume P = pressure E = total energy of the material
Formation Energy	Formation Energy (E_f): $E\_f = [E\_total(A_xB_Y) - x*\mu\_A - y*\mu\_B] / (x + y)$	E_total(AxBy) = total DFT energy of compound AxBy μA = chemical potential of element A μB = chemical potential of element B x = number of atoms of A y = number of atoms of B

Loss Function

Training Loss Function: Mean Squared Error (MSE)

Mean Squared Error (MSE): $MSE = (1/n) \times \Sigma (y_i - \hat{y}_i)^2$

Parameters:

n = total number of data points

y_i = actual (true) value

$\hat{y}_i$ = predicted value

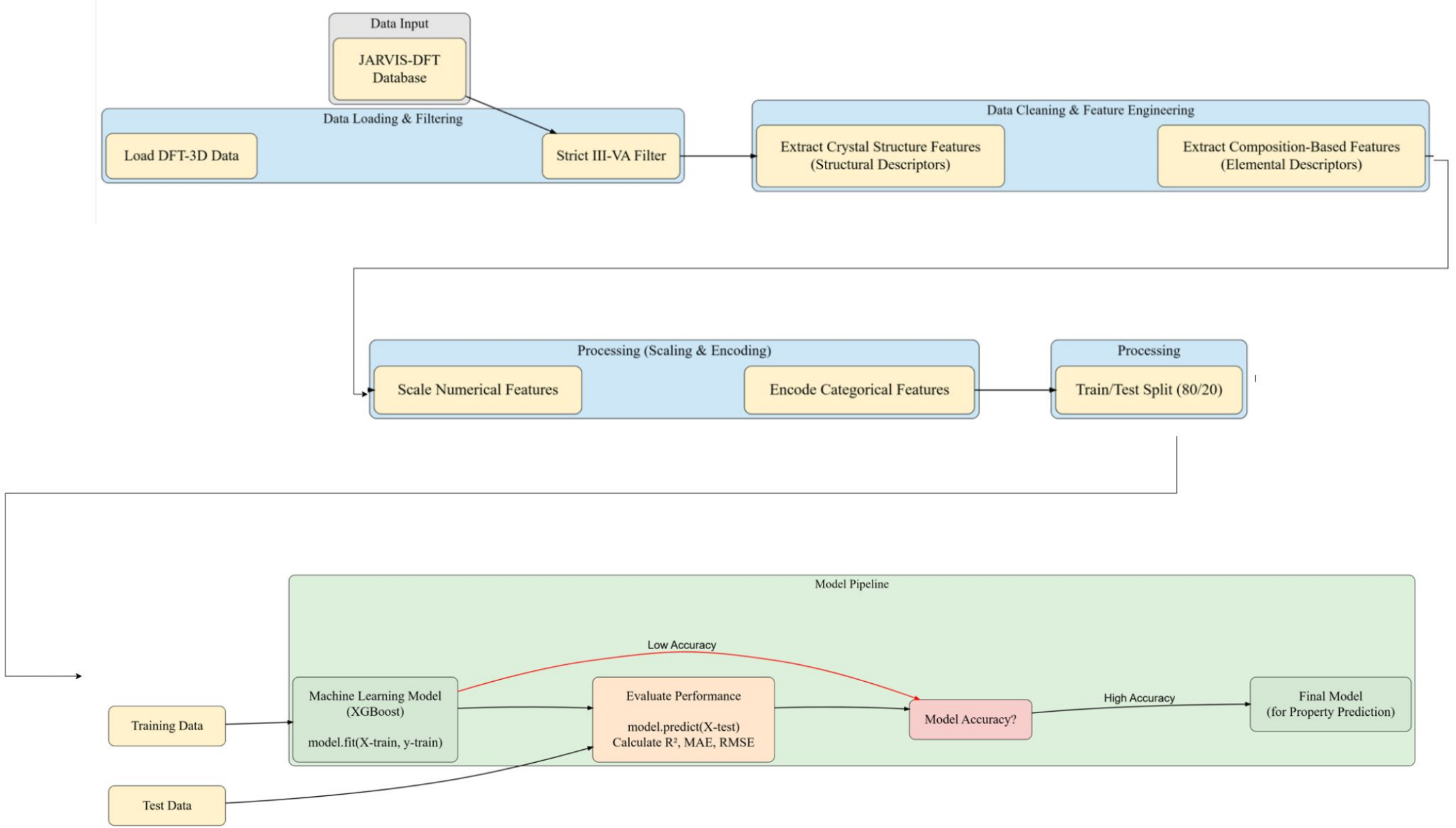
Why MSE?

- Penalizes larger errors more heavily due to squaring.
- Encourages predictions to be close to true values on average.
- Smooth gradient for optimization → better convergence in tree-based models.

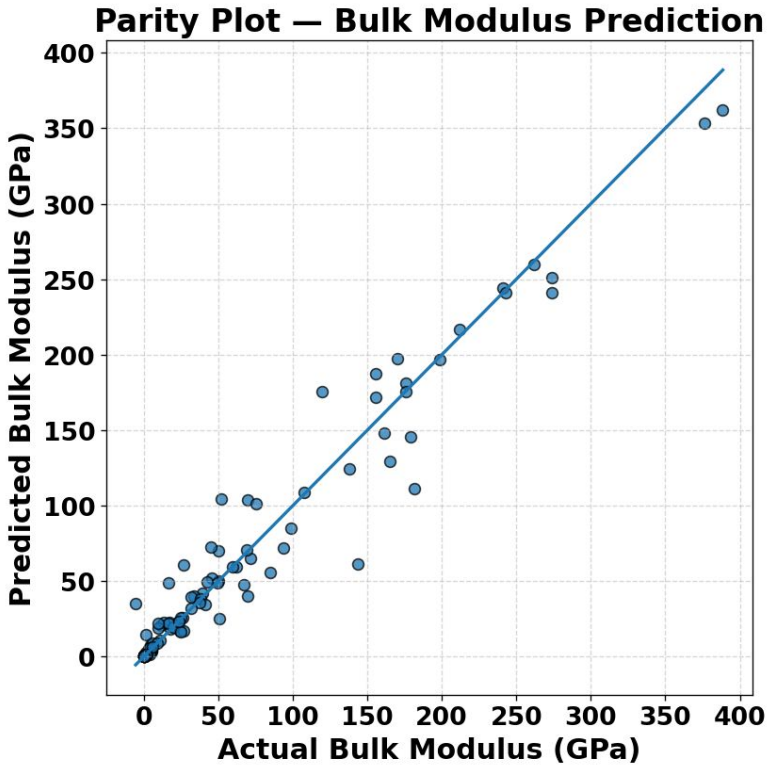
Evaluation Metrics

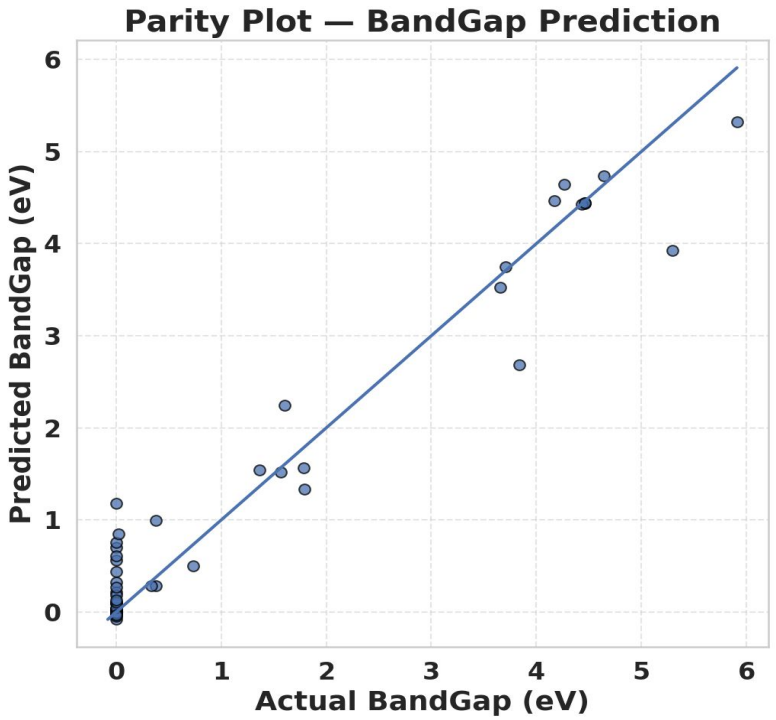
- R^2 (Coefficient of Determination): $R^2 = 1 - [\ \Sigma (y_i - \hat{y}_i)^2 / \Sigma (y_i - \bar{y})^2\ ]$
- Mean Absolute Error (MAE): $MAE = (1/n) \times \Sigma\ |y_i - \hat{y}_i|$
- Root Mean Squared Error (RMSE): $RMSE = \sqrt{[\ (1/n) \times \Sigma (y_i - \hat{y}_i)^2\ ]}$

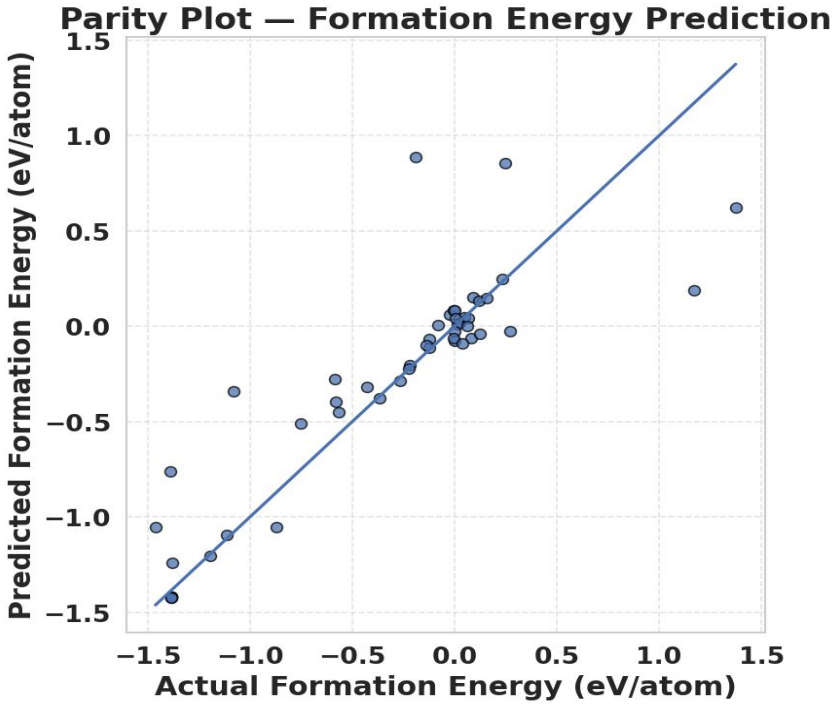
Pipeline for Predicting Target Properties



Parity Plots & Accuracy







	Train R2	Test R2	MAE	RMSE
Bandgap (eV)	0.994	0.949	0.2689	0.4362
Bulk Modulus (GPa)	0.999	0.946	16.971	26.446
Formation Energy (eV/atom)	0.996	0.736	0.153	0.334

Conclusions

- To overcome the high computational cost and time required by DFT for screening new IIIA–VA materials, a machine-learning-based predictive framework using XGBoost has been developed.

- We constructed ML models to estimate Band Gap, Formation Energy, and Bulk Modulus using reliable JARVIS-DFT data and carefully engineered structural and compositional features.

- The predicted results show strong agreement with DFT-reported values, demonstrating that the proposed ML approach can efficiently capture key material property trends while drastically reducing computation time.

- This framework provides a promising pathway for rapid materials discovery and optimization in semiconductor applications, enabling large-scale screening of unexplored III–V compounds.