Supporting Information:

Toward Accelerating Rare-Earth Metal Extraction Using Equivariant Neural Networks

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Table S1: Charge of the four fundamental ligands present in the dataset: hydroxypyridinone (HOPO), hydroxypyridinone's sulfur analogue (thio-HOPO), catecholamide (CAM) and catecholamide's sulfur analogue (thio-CAM).

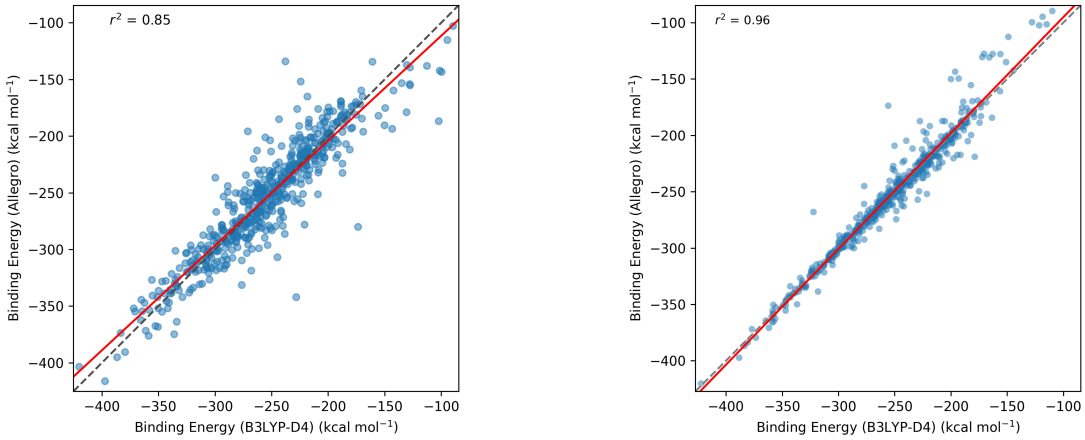
Ligand	Charge
HOPO	-1
Thio-HOPO	-1
CAM	-2
Thio-CAM	-2

Table S2: Spin multiplicity of the 16 rare-earth element metals (Sc, Y, and lanthanides (La–Lu)) present in the dataset.

Metal Cation	Spin Multiplicity
La^{3+}	1
Y^{3+}	1
Ce^{3+}	2
Pr^{3+}	3
Nd^{3+}	4
Pm^{3+}	5
Sm^{3+}	6
Eu^{3+}	7
Gd^{3+}	8
Tb^{3+}	7
Dy^{3+}	6
Ho^{3+}	5
Er^{3+}	4
Tm^{3+}	3
Yb^{3+}	2
Lu^{3+}	1

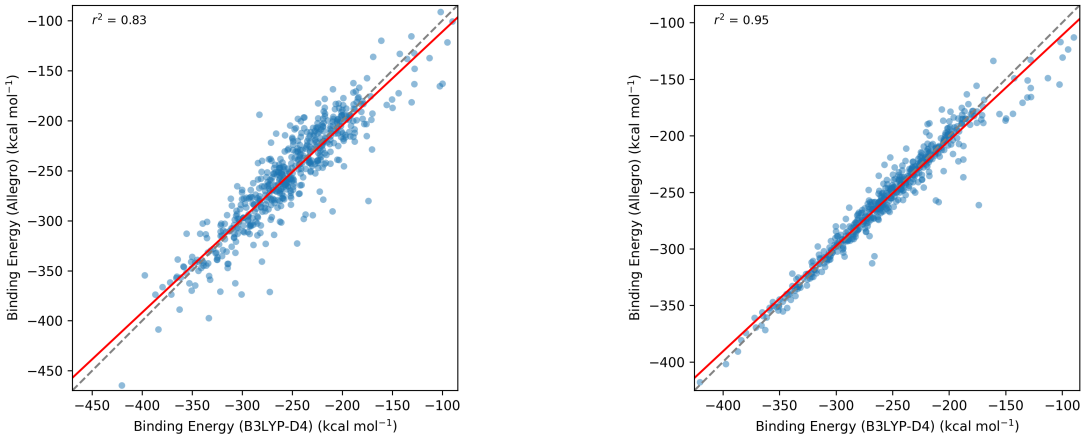
Table S3: Hyperparameters used in the Allegro model trained on absolute energies, binding energies and delta-ML energies.

Hyperparameters	**Allegro Model**
Number of layers	2
l_{max}	2
2-body latent multi-layer perceptron (MLP)	[8, 16, 32, 64]
Latent MLP	[8, 16, 32, 64]
Final edge-energy MLP	[16]
Tensor features (env embedded multiplicity)	2 / 4



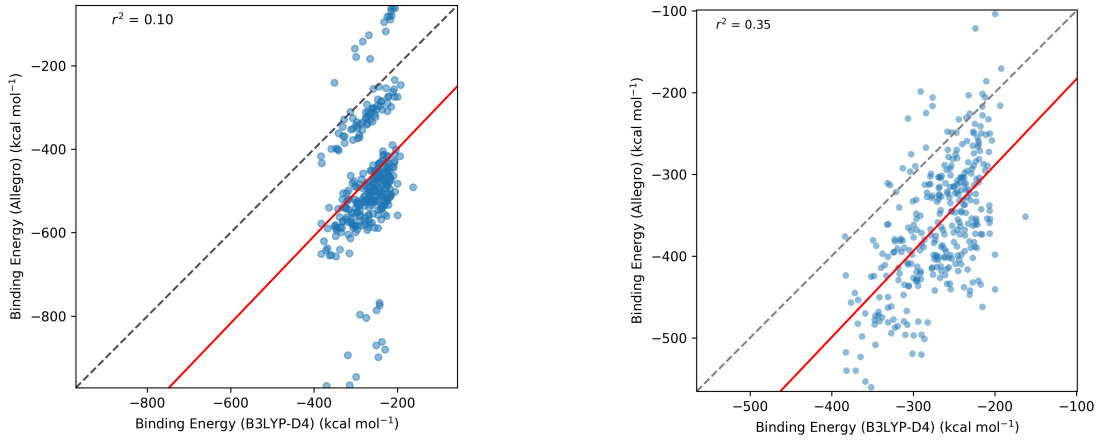
(a) **(b)**

Figure S1: Parity plots comparing binding energies predicted by the Allegro model (features = 2) against DFT-calculated values (B3LYP-D4) for the test set. (a) Results using strategy 1, where absolute energies were predicted first ($r^2 = 0.85$). (b) Results using strategy 2, where binding energies were predicted directly ($r^2 = 0.96$). Binding energies are in kcal mol^{-1}. The dashed black line represents perfect correlation (y=x), while the solid red line indicates the line of best fit.



(a) **(b)**

Figure S2: Parity plots comparing binding energies predicted using the Allegro (features = 2) Δ-ML approach against DFT-calculated values (B3LYP-D4) for the test set. (a) Results using Δ-ML strategy 1, where the correction was learned on absolute energies ($r^2 = 0.83$). (b) Results using Δ-ML strategy 2, where the correction was learned directly on binding energies ($r^2 = 0.95$). Binding energies are in kcal mol^{-1}. The dashed black line represents perfect correlation (y=x), while the solid red line indicates the line of best fit.



(a) **(b)**

Figure S3: Parity plots comparing binding energies for the out-of-sample HDEV test set predicted using Allegro (features = 4) against DFT-calculated values (B3LYP-D4). (a) Results using strategy 1, where absolute energies were predicted first ($r^2 = 0.10$). (b) Results using Δ-ML strategy 1, where the correction was learned on absolute energies ($r^2 = 0.35$). Binding energies are in kcal mol^{-1}. The dashed black line represents perfect correlation (y=x), while the solid red line indicates the line of best fit.

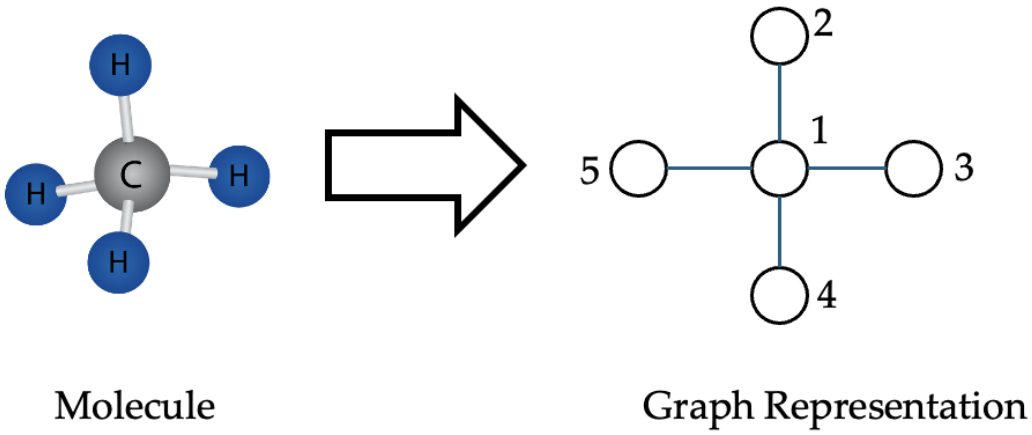


Figure S4: Schematic of a Graph Neural Network (GNN) for chemistry. A molecule (methane, left) is represented as a graph (right), where atoms are treated as nodes and bonds as edges. The figure also contrasts the common per-atom energy decomposition ($E = \sum_i E_i$) with the per-pair energy decomposition ($E = \sum_i \sum_j E_{ij}$) used by the Allegro architecture.