

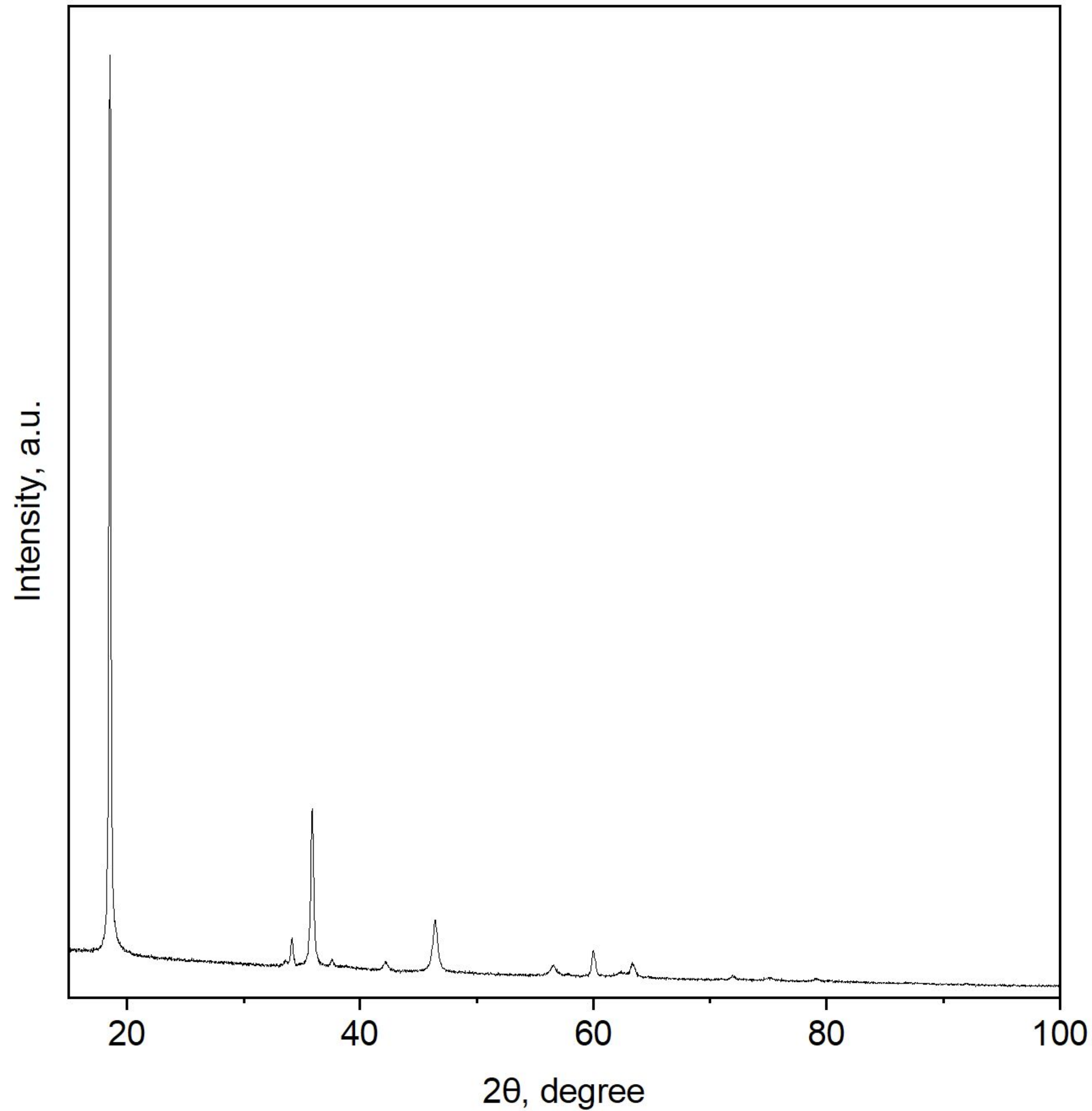
**Crystallography and Crystal Chemistry
IX International School-Conference of
Young Scientists 2025**

***Machine-learning XRD Patterns
analysis***

Arseniy Burov

Skoltech Center for
Energy Science
and Technology
Energy

November, 2025



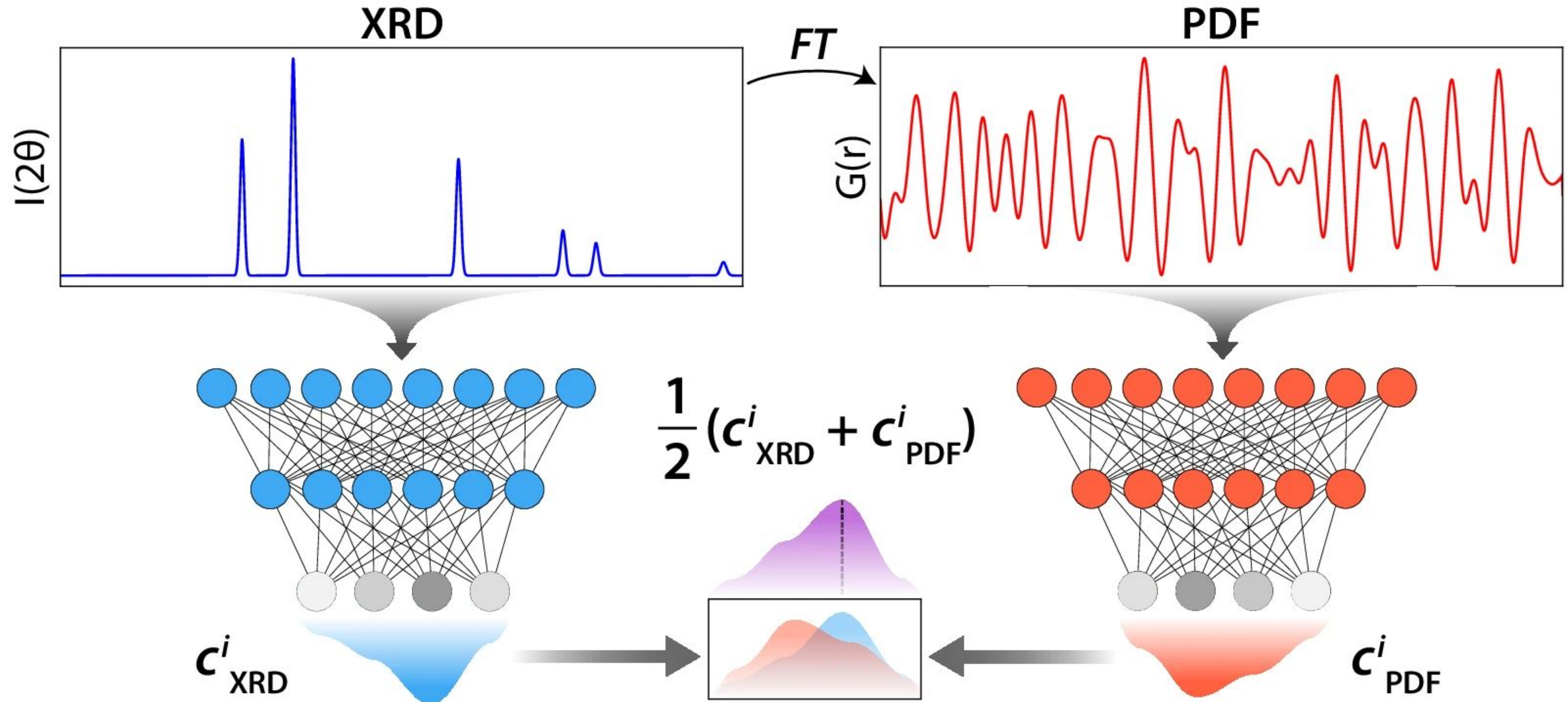
Some unknown phase from
the experiment.

We have XRD pattern?

How to identify it?

Crystal structure representation for NN

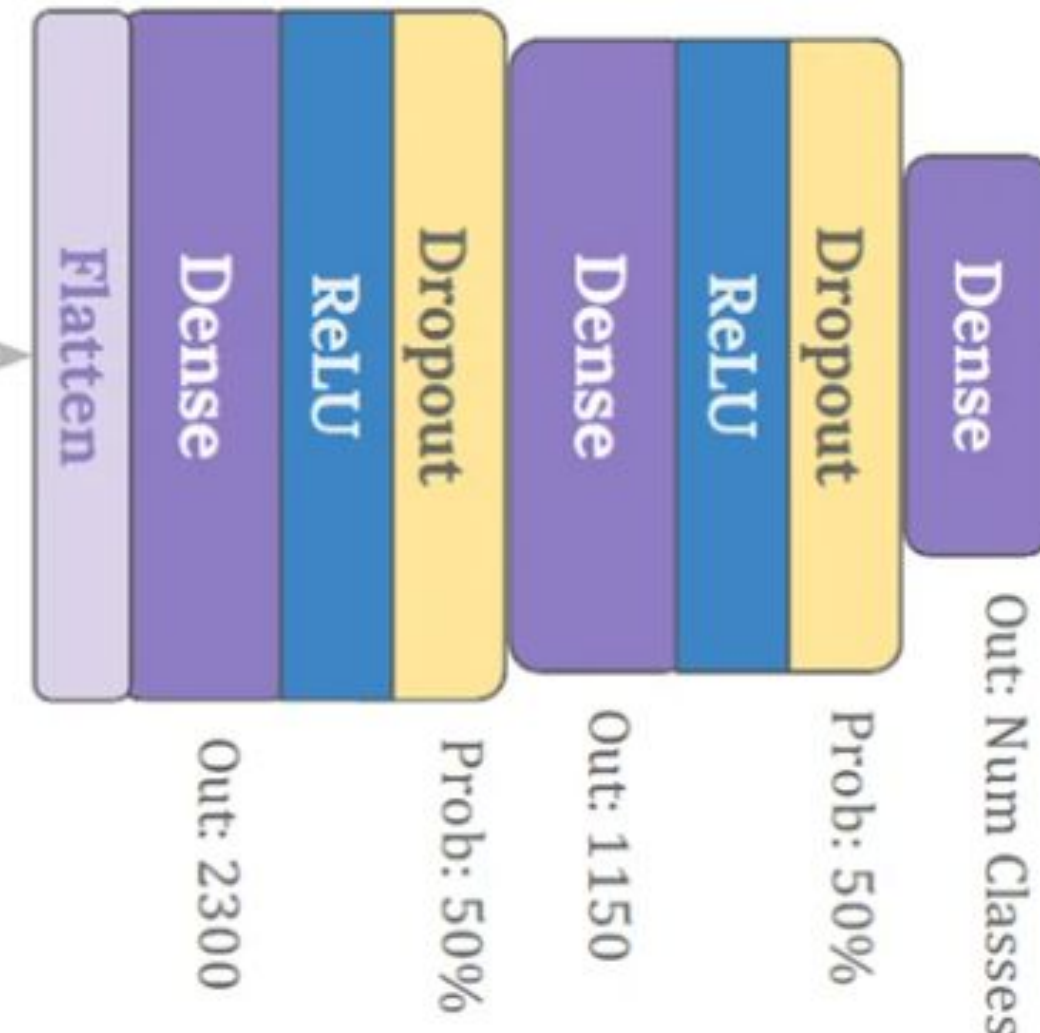
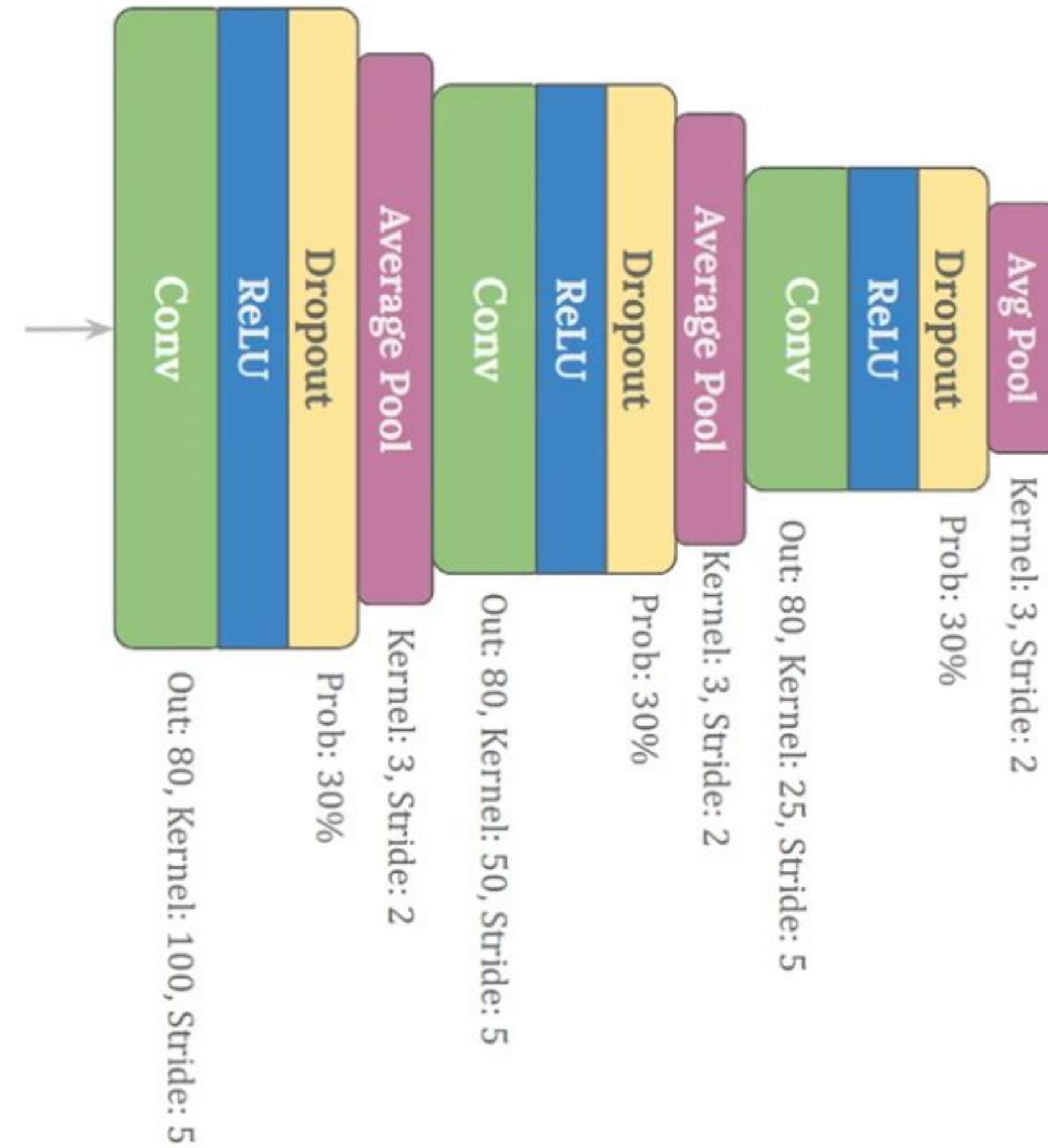
Szymanski, N. (2024). *npj Computational Materials*, 10(45).



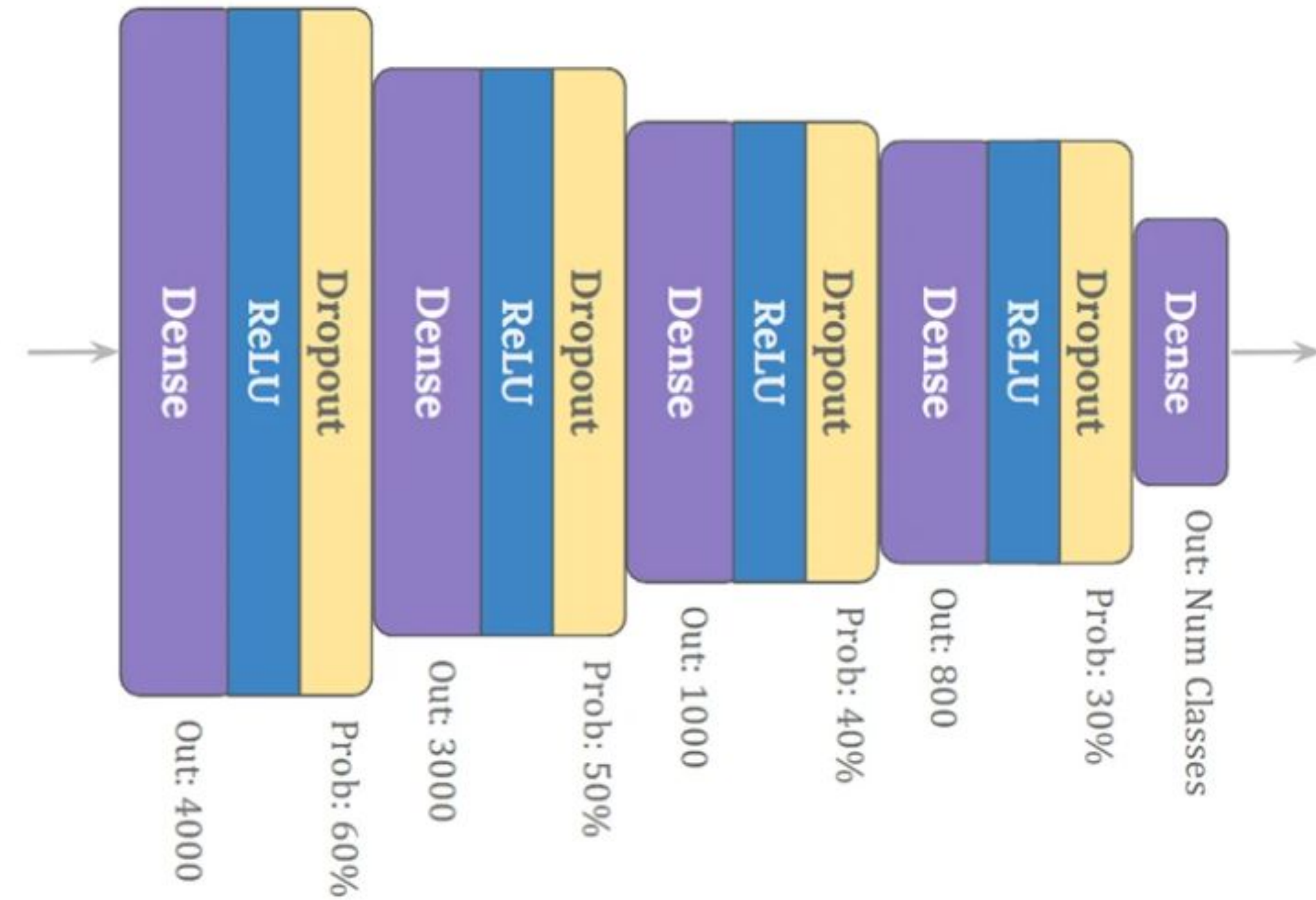
Given a pattern to be classified, a Fourier transform (FT) is used to calculate its virtual PDF.

Types on NN used for XRD detection

a) SCNN

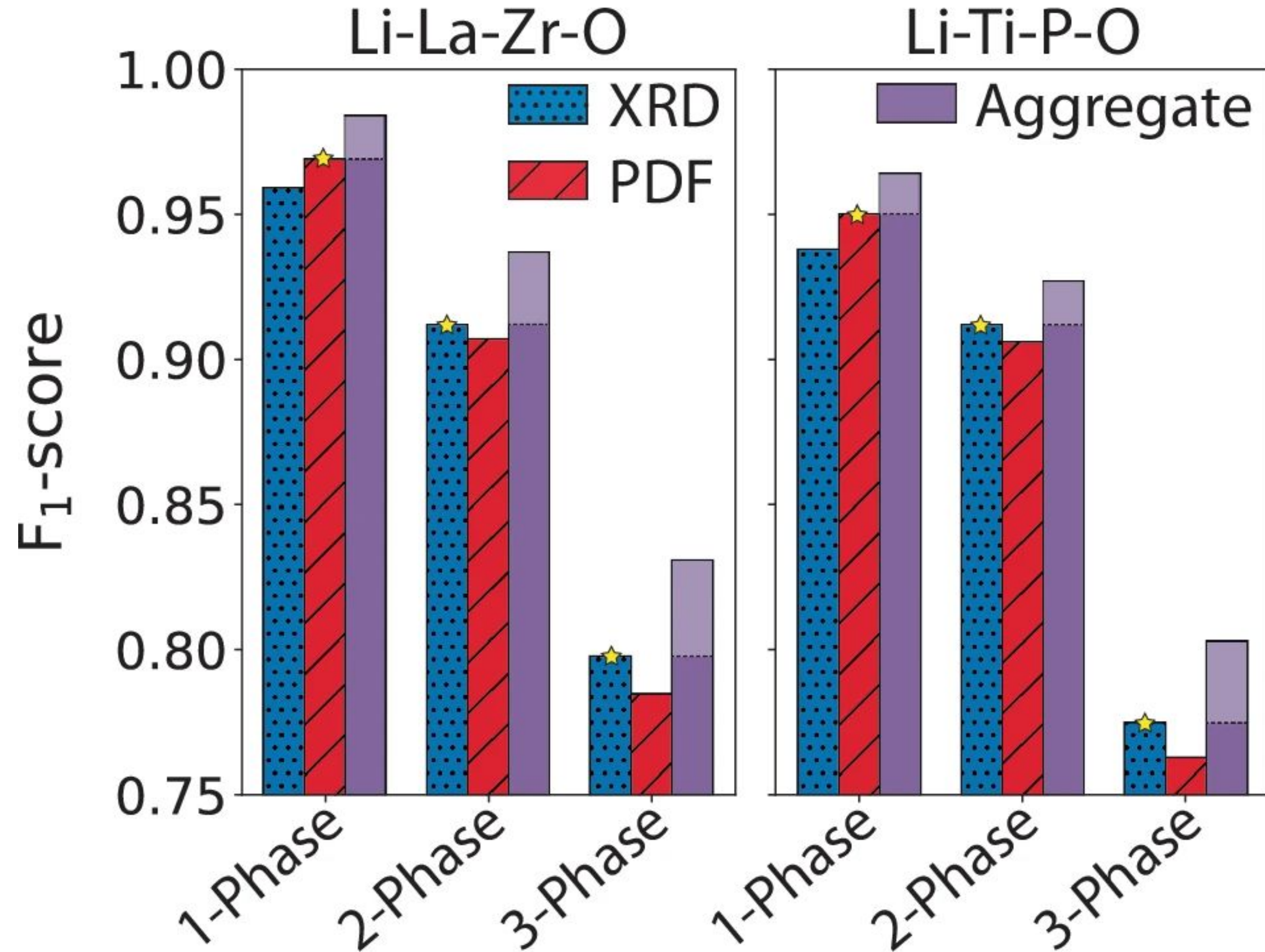


b) MLP



Salgado, E. (2023). *npj Computational Materials*, 9(214).

Model architecture specifications used. We have a Standard convolutional neural network (SCNN) and b multi-layer perceptron (MLP) architectures.



Example from “cutting-edge” science

Article | [Open access](#) | Published: 29 November 2023

An autonomous laboratory for the accelerated synthesis of novel materials

[Nathan J. Szymanski](#), [Bernardus Rendy](#), [Yuxing Fei](#), [Rishi E. Kumar](#), [Tanjin He](#), [David Milsted](#),
[Matthew J. McDermott](#), [Max Gallant](#), [Ekin Dogus Cubuk](#), [Amil Merchant](#), [Haegyeom Kim](#), [Anubhav Jain](#), [Christopher J. Bartel](#), [Kristin Persson](#), [Yan Zeng](#) ✉ & [Gerbrand Ceder](#) ✉

[Nature](#) **624**, 86–91 (2023) | [Cite this article](#)

215k Accesses | **553** Citations | **1097** Altmetric | [Metrics](#)

Example from “cutting-edge” science

Challenges in high-throughput inorganic material prediction and autonomous synthesis

08 January 2024, Version 1

Review

[Josh Leeman](#) , [Yuhan Liu](#) , [Joseph Stiles](#), [Scott Lee](#), [Prajna Bhatt](#) ,
[Leslie Schoop](#) , [Robert Palgrave](#)

[Show author details](#) 

Post-analysis of the results

| Claimed Phases | 1 | 2 | 3 | 4 | Claimed Phases | 1 | 2 | 3 | 4 |
|--|---|---|---|---|--|---|---|---|---|
| Ba ₂ ZrSnO ₆ | X | X | X | | Mg ₃ MnNi ₃ O ₈ | X | | X | |
| Ba ₆ Na ₂ Ta ₂ V ₂ O ₁₇ | X | | X | | Mg ₃ NiO ₄ | | X | X | |
| Ba ₆ Na ₂ V ₂ Sb ₂ O ₁₇ | X | | | | MgCuP ₂ O ₇ | | X | X | |
| CaCo(PO ₃) ₄ | | | X | | MgNi(PO ₃) ₄ | X | | X | |
| CaFe ₂ P ₂ O ₉ | | | | | MgTi ₂ NiO ₆ | | | X | |
| CaMn(PO ₃) ₄ | | | X | | MgTi ₄ (PO ₄) ₆ | | | | X |
| CaNi(PO ₃) ₄ | | | X | | MgV ₄ Cu ₃ O ₁₄ | X | X | X | |
| FeSb ₃ Pb ₄ O ₁₃ | | | X | | Mn ₂ VPO ₇ | X | | X | |
| Hf ₂ Sb ₂ Pb ₄ O ₁₃ | | | X | | Mn ₄ Zn ₃ (NiO ₆) ₂ | | | X | |
| InSb ₃ Pb ₄ O ₁₃ | | | X | | MnAgO ₂ | X | | | X |
| K ₂ TiCr(PO ₄) ₃ | | | X | | Na ₃ Ca ₁₈ Fe(PO ₄) ₁₄ | X | | | |
| K ₄ MgFe ₃ (PO ₄) ₅ | X | | | | Na ₇ Mg ₇ Fe ₅ (PO ₄) ₁₂ | X | | | |
| K ₄ TiSn ₃ (PO ₅) ₄ | X | | | | NaCaMgFe(SiO ₃) ₄ | | X | X | |
| KBaPrWO ₆ | X | | | | NaMnFe(PO ₄) ₂ | X | | | |
| KMn ₃ O ₆ | X | X | X | | Sn ₂ Sb ₂ Pb ₄ O ₁₃ | | | X | |
| KNaP ₆ (PbO ₃) ₈ | X | X | X | | Y ₃ In ₂ Ga ₃ O ₁₂ | X | | | X |
| KNaTi ₂ (PO ₅) ₂ | | | X | | Zn ₂ Cr ₃ FeO ₈ | | | X | |
| KPr ₉ (Si ₃ O ₁₃) ₂ | X | X | | | Zr ₂ Sb ₂ Pb ₄ O ₁₃ | | | X | |

Error 1 – is a very poor fit, such that the fitted model is meaningless.

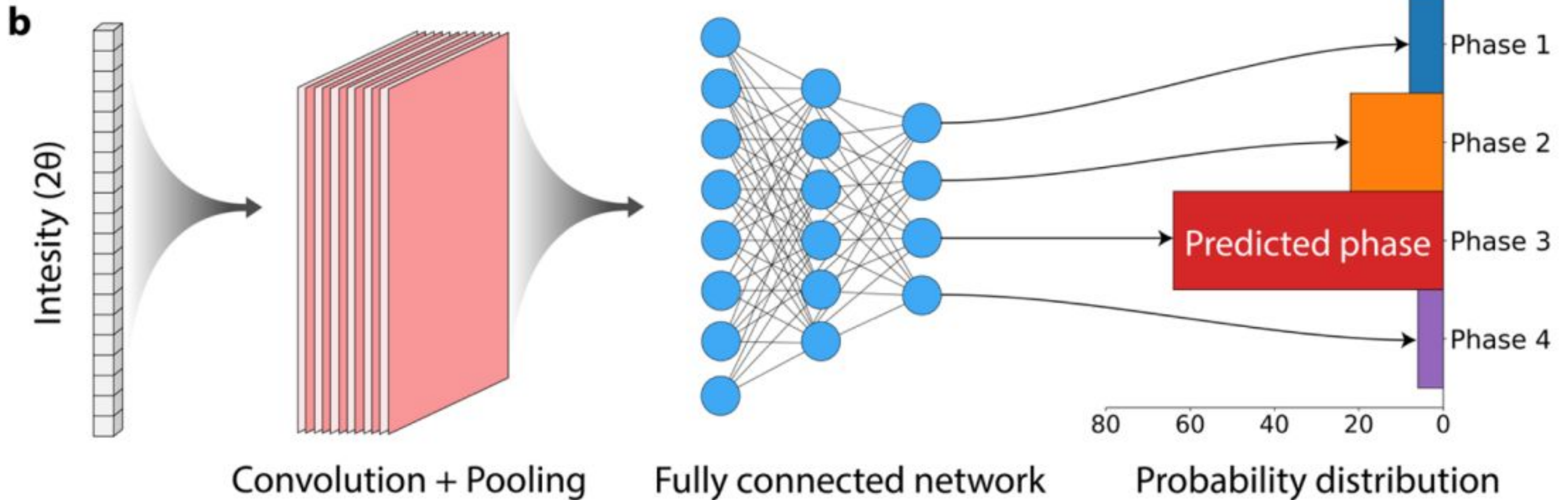
Error 2 – where a different CIF has been used for refinement compared with that in the paper and in the Materials Project.

Error 3 – where the predicted structure has ordered cations but there is no evidence for order, and a known disordered version of the compound exists.

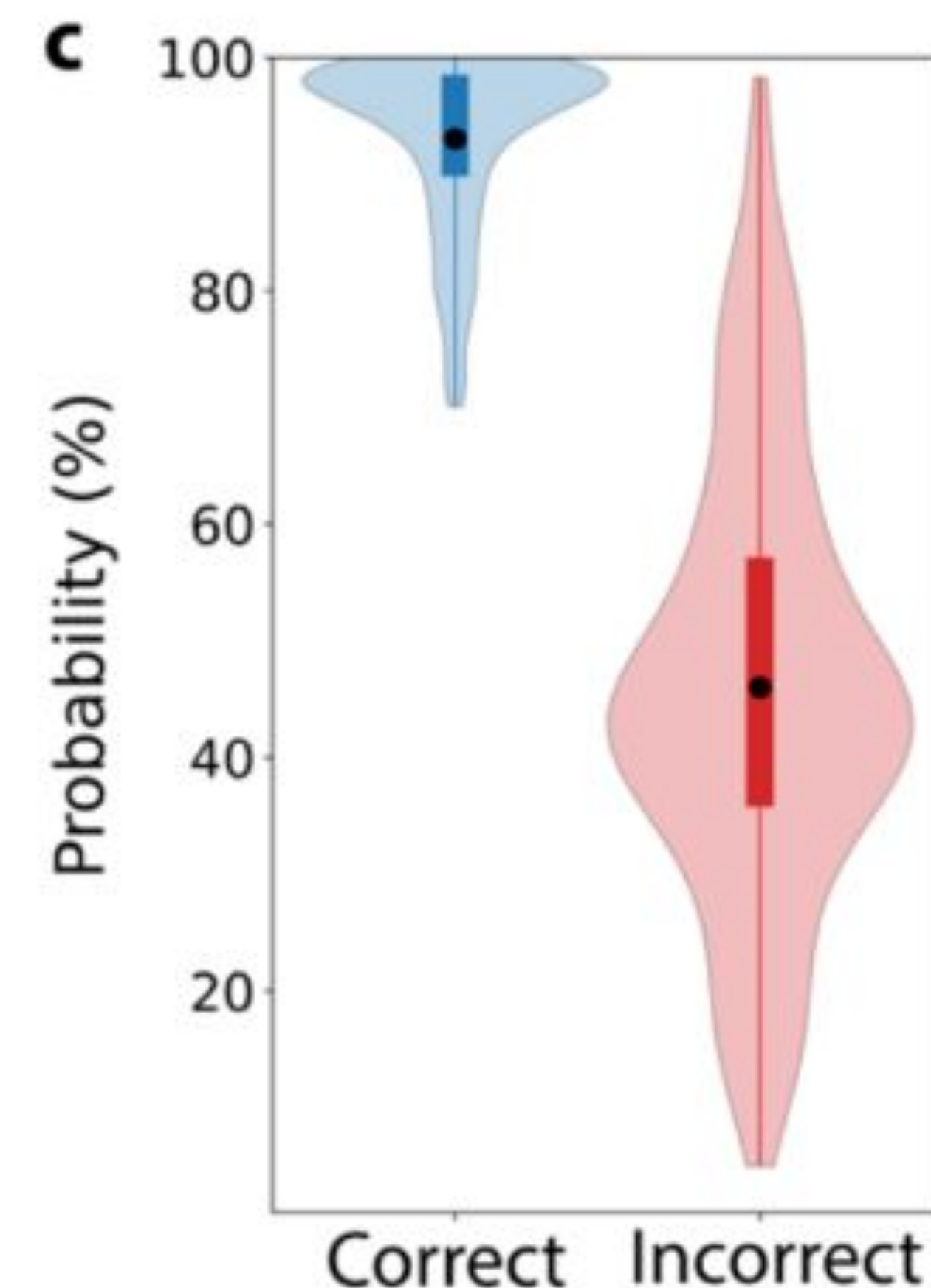
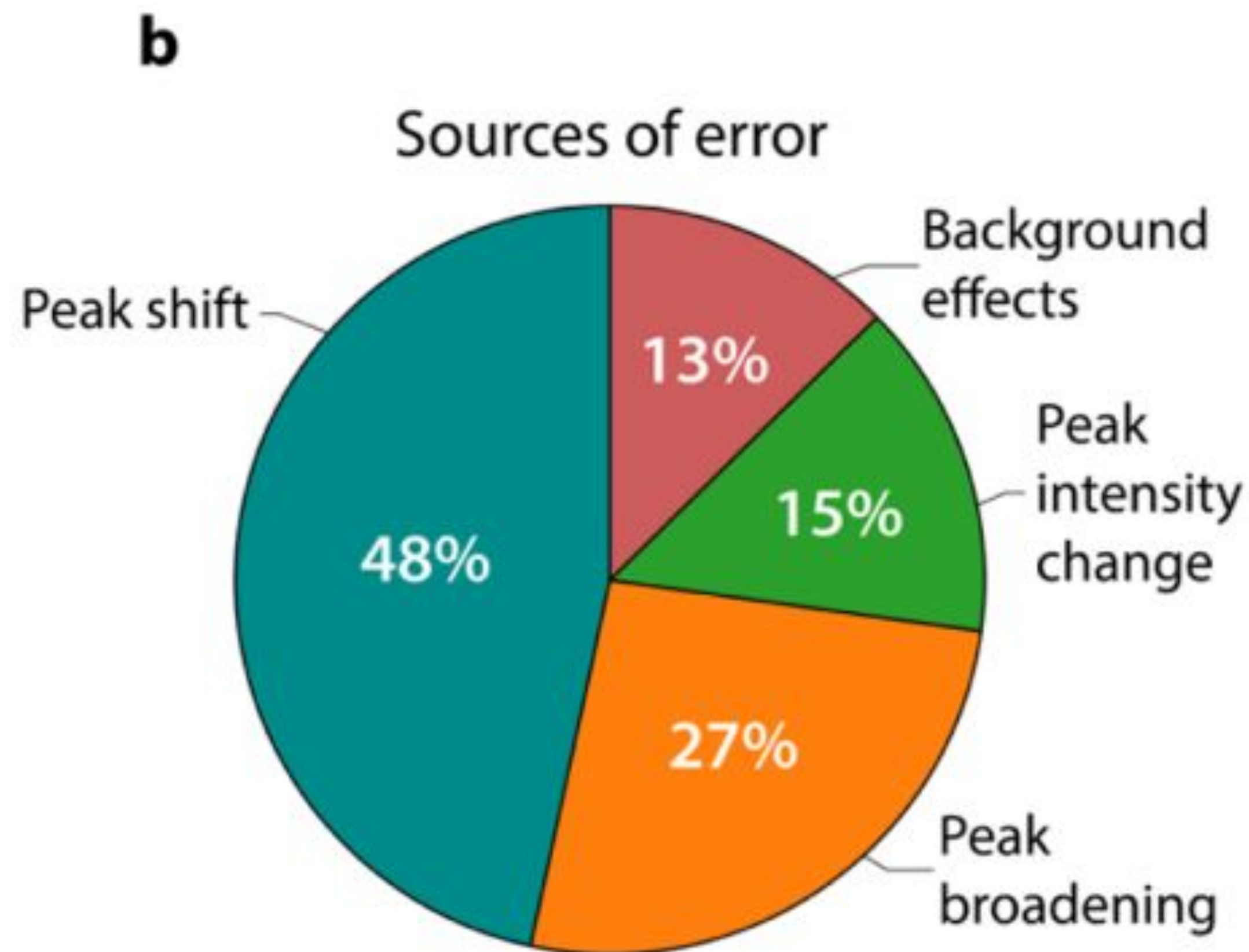
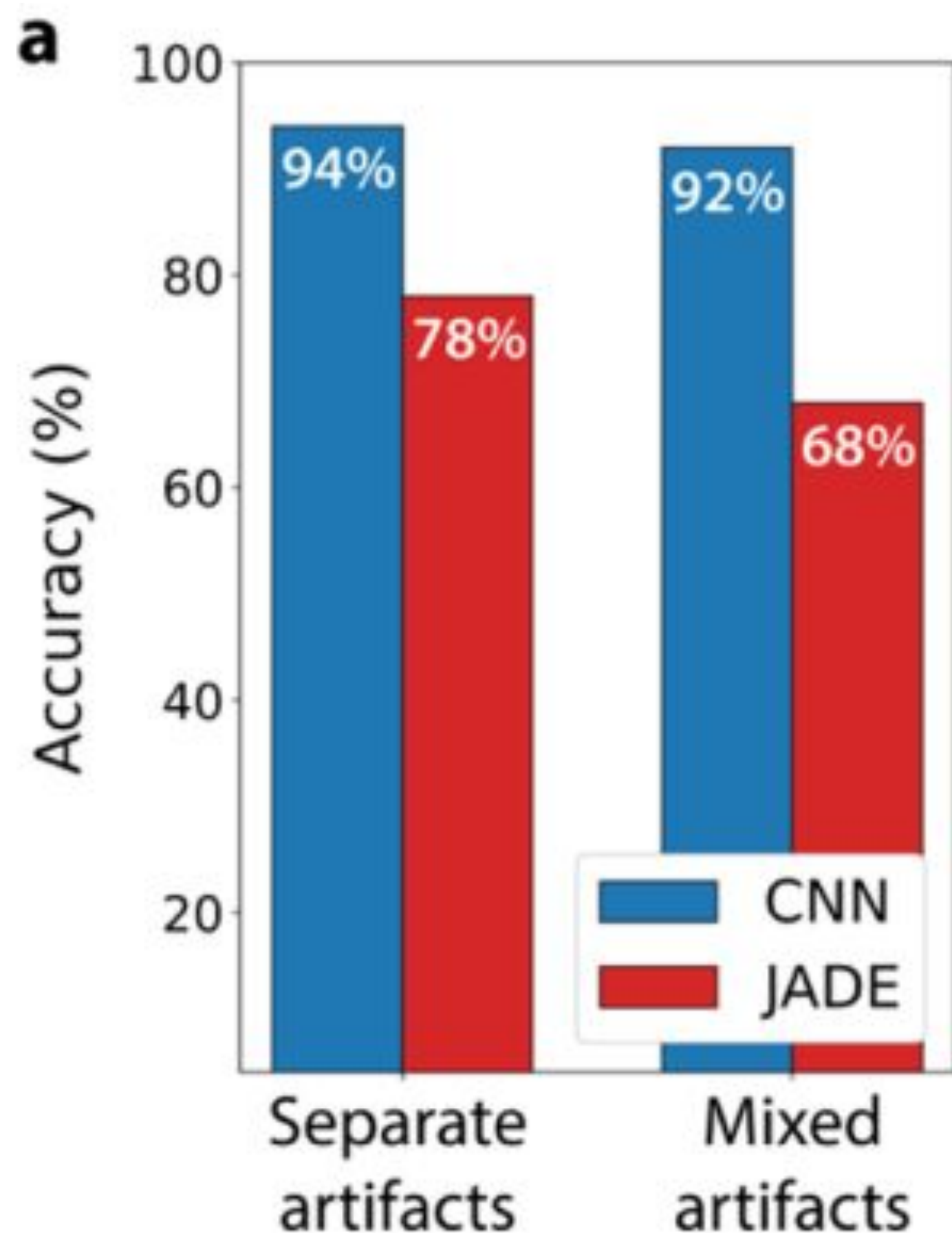
Error 4 – where the compound is correctly identified but is already reported.

Pre-trained model of XRD-AutoAnalyzer

Was pretrained on the Li–Mn–Ti–O–F chemical space (46 structures)



Pre-trained model of XRD-AutoAnalyzer



Training set: 16,800 spectra

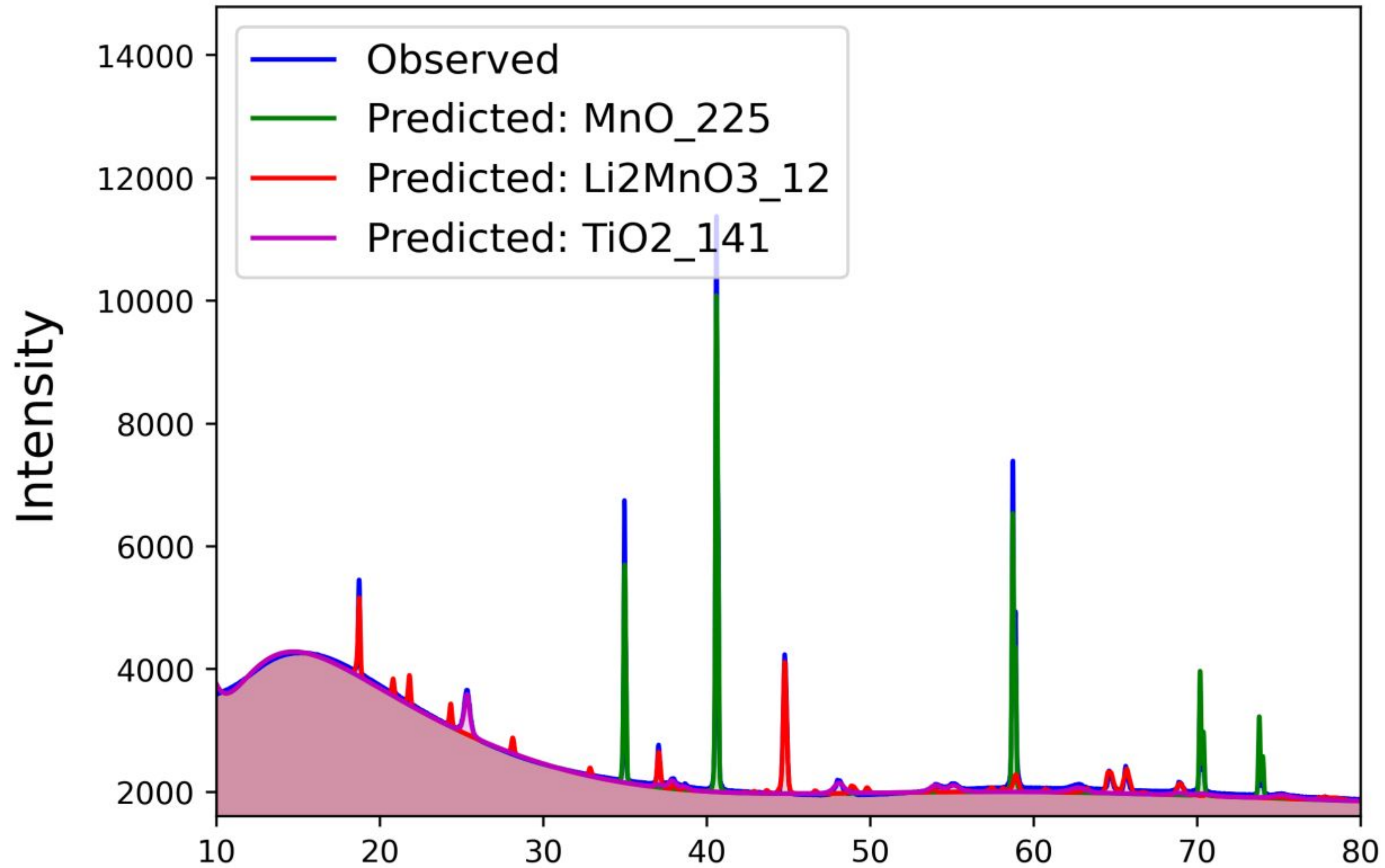
- ✓ Single-phase
- ✓ Stoichiometric
- ✓ Separate artifacts
- ✓ Peak perturbations
- ✗ Background effects
- ✗ Mixed artifacts

Test set: 4,200 spectra

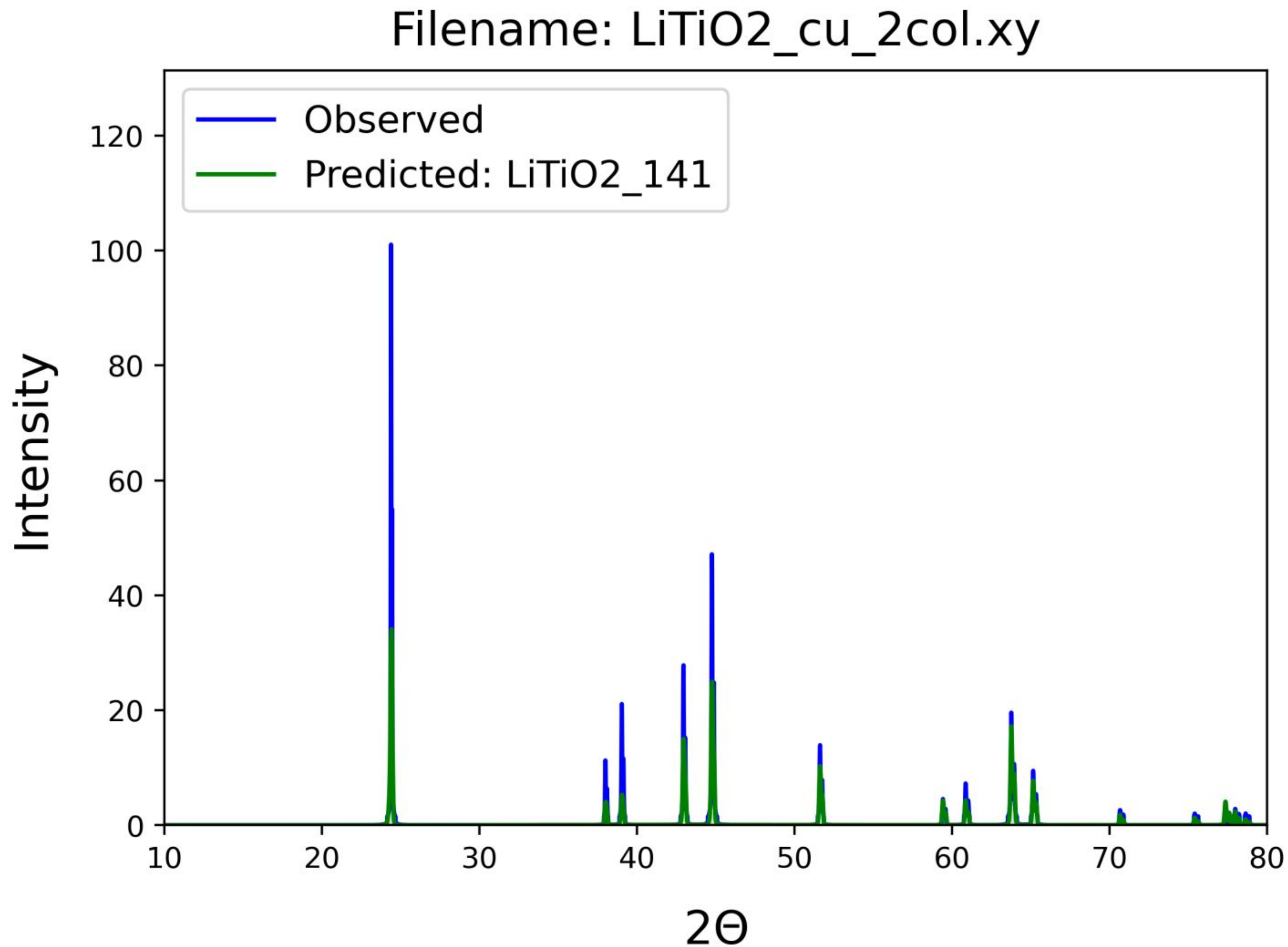
- ✓ Single-phase
- ✓ Stoichiometric
- ✓ Separate artifacts
- ✓ Peak perturbations
- ✓ Background effects
- ✓ Mixed artifacts

Original chemical space: Li–Mn–Ti–O–F (multi-phase)

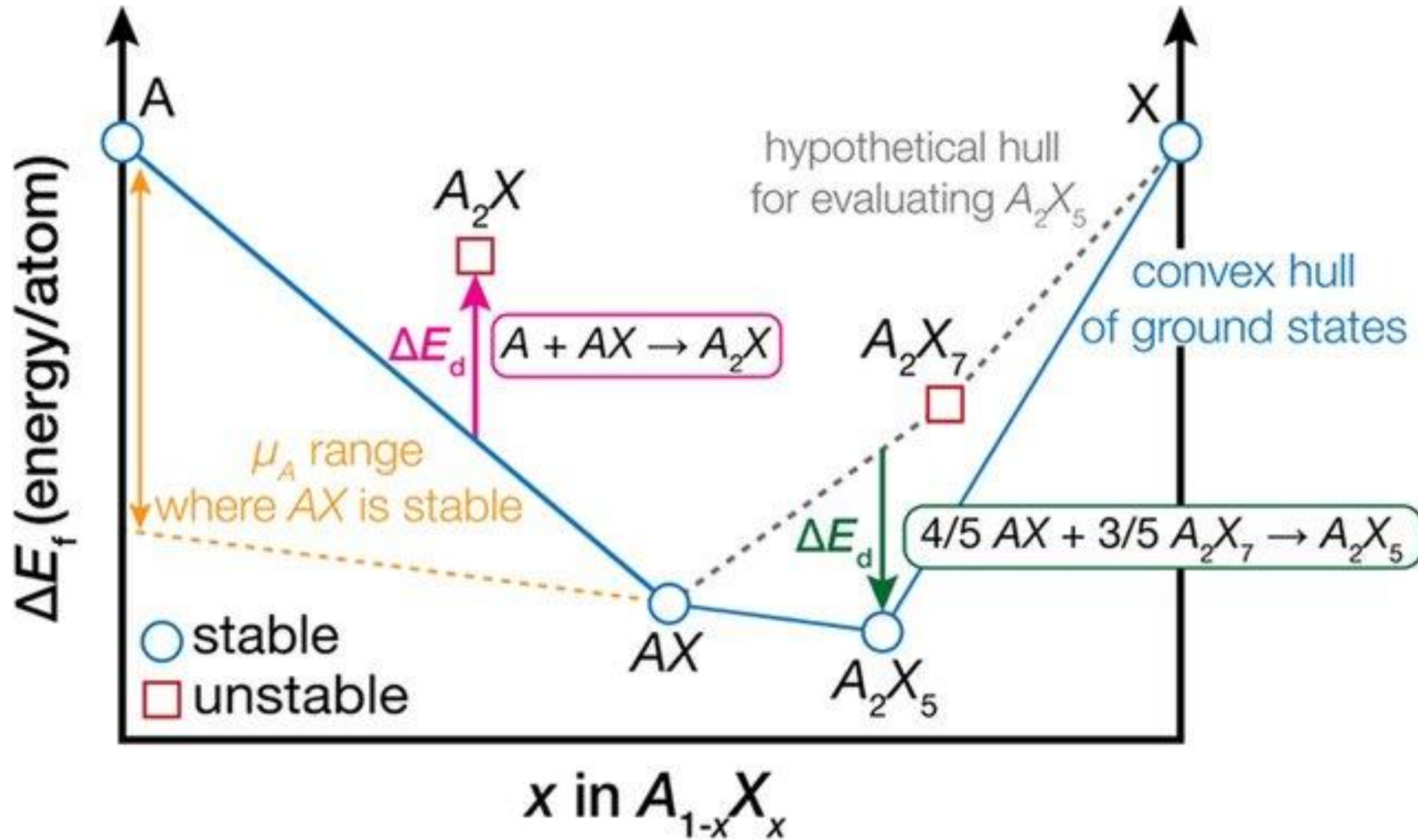
Filename: Li2MnO3+MnO+TiO2.xy



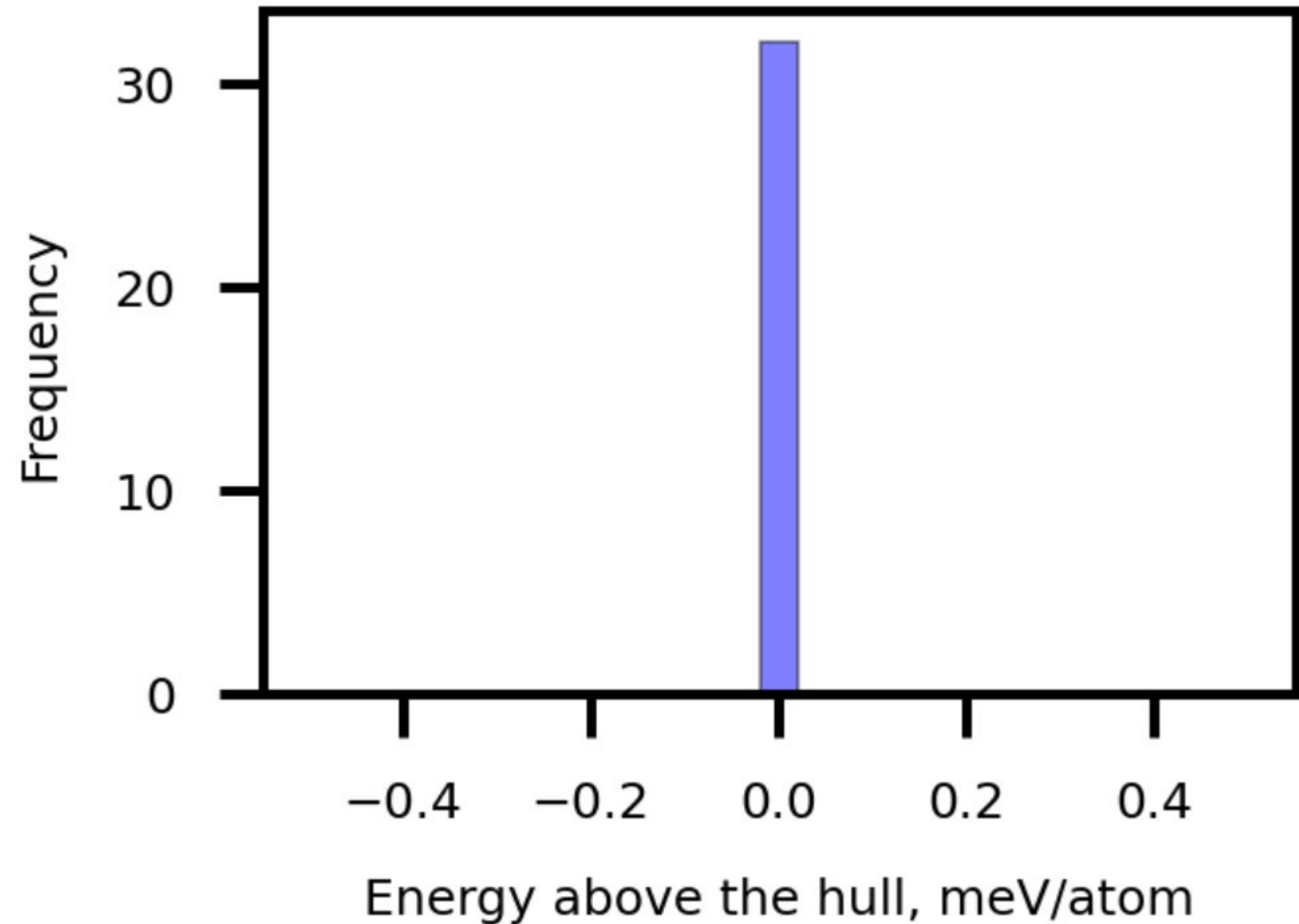
Original chemical space: Li–Mn–Ti–O–F (lab sample)



How to evaluate the stability of a structure?

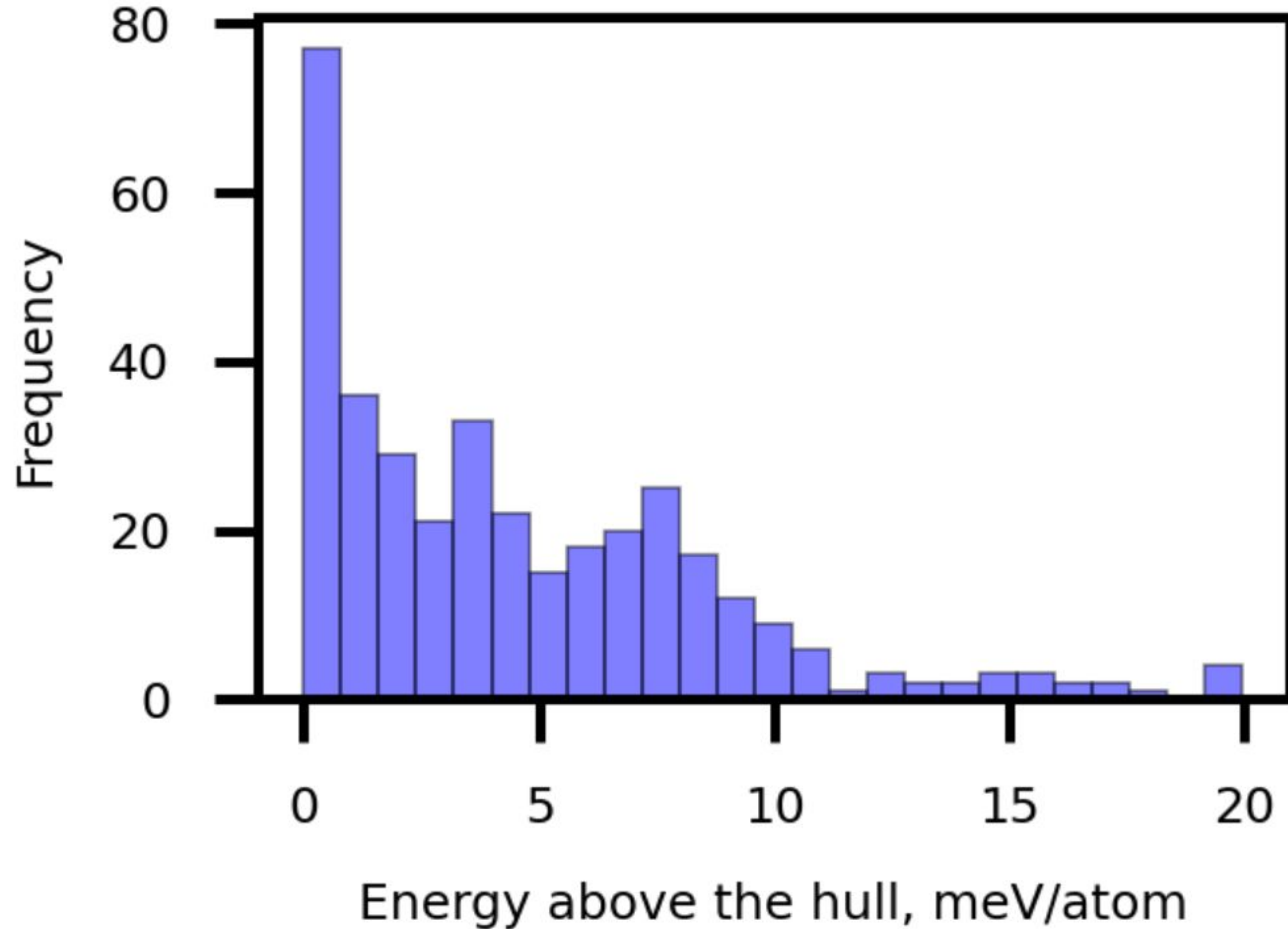


Structure mining from Materials Project: Li–Ni–O–H–F



Stable phases: 32 samples with energy above the hull = 0 eV/atom

Structure mining from Materials Project: Li-Ni-O-H-F



Metatable phases: 239 samples with energy above the hull = 0 eV/atom

Structures in the training dataset

Li-Ni-O-H-F chemical space (362 entries):

MP phases with $E_{\text{above_the_hull}} < 0.02$ eV/atom

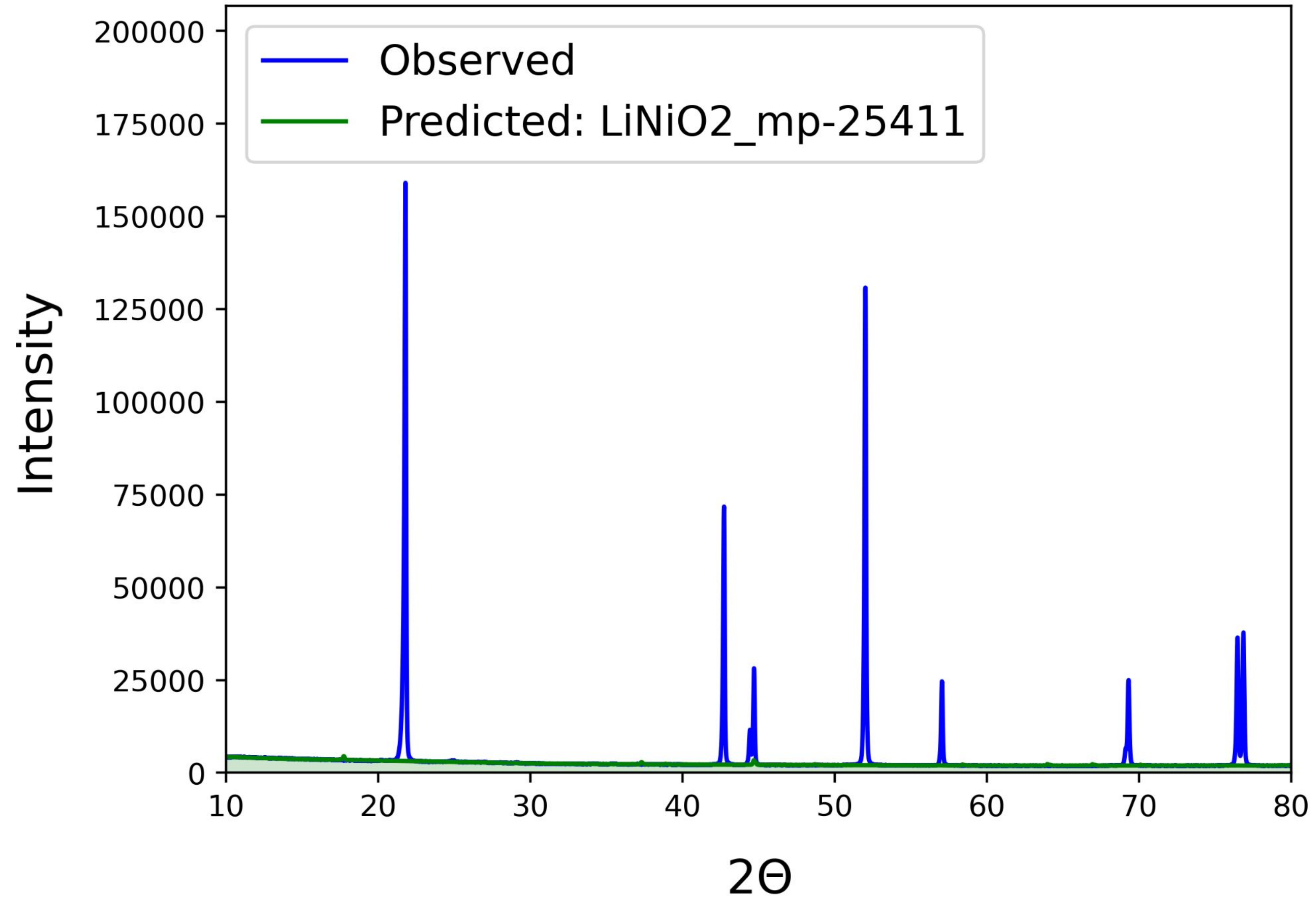
```
F2_mp-1525632.cif HF_mp-1536913.cif KHO_mp-626716.cif 'Li11(NiO2)12_mp-38676.cif' 'Li5(NiO2)6_mp-690572.cif' LiNiO2_mp-25411.cif Na2O2_mp-2340.cif NaH9O5_mp-505077.cif Na_mp-982370.cif
F2_mp-561203.cif K2H5F7_mp-29330.cif KHO_mp-626785.cif Li11Ni13024_mp-758517.cif Li5Ni7012_mp-756931.cif LiNiO2_mp-752850.cif Na2O9_mp-1204051.cif NaH9O5_mp-625378.cif 'Ni(HO)2_mp-1180084.cif'
F2_mp-561367.cif K2Li3NiO4_mp-774432.cif KHO_mp-642817.cif Li13Ni15028_mp-757347.cif Li5NiO4_mp-771876.cif LiNiO2_mp-770635.cif Na2O_mp-2352.cif NaHF2_mp-27837.cif 'Ni(HO)2_mp-1275121.cif'
F2_mp-760482.cif K2NaNiF6_mp-556757.cif KH_mp-24084.cif Li13Ni15028_mp-766878.cif 'Li7(NiO2)8_mp-690528.cif' LiNiO2_mp-849241.cif 'Na3(NiO2)5_mp-759923.cif' NaHO_mp-23891.cif 'Ni(HO)2_mp-27912.cif'
H2O_mp-1974803.cif K2NiF4_mp-556546.cif 'KLi2(HO)3_mp-1188395.cif' Li13Ni9022_mp-769473.cif 'Li7(NiO2)9_mp-757736.cif' LiNiO2_mp-850062.cif Na3NiF6_mp-554649.cif NaHO_mp-23940.cif 'Ni(HO)2_mp-625074.cif'
H2O_mp-24043.cif K2NiF6_mp-605034.cif KLiO_mp-559612.cif Li17Ni11028_mp-757655.cif 'Li7(NiO2)9_mp-757736.cif' LiNiO2_mp-865631.cif Na3NiO3_mp-755725.cif NaHO_mp-626000.cif Ni3O4_mp-656887.cif
H2O_mp-557082.cif K2NiO2_mp-19252.cif KNa2_mp-570786.cif Li19Ni23042_mp-698842.cif 'Li9(NiO2)10_mp-769454.cif' LiNiO2_mp-866271.cif Na4(NiO2)5_mp-753301.cif NaHO_mp-626778.cif NiF2_mp-556324.cif
H2O_mp-558226.cif K2O2_mp-2672.cif KNaO_mp-6948.cif Li2Ni507_mp-754083.cif LiF_mp-1138.cif LiO8_mp-1232999.cif 'Na4(NiO2)9_mp-764295.cif' NaH_mp-23870.cif NiF2_mp-559798.cif
H2O_mp-558958.cif K2O_mp-971.cif KNiF3_mp-560976.cif Li2NiF4_mp-35759.cif LiH3O2_mp-27281.cif LiO8_mp-1235059.cif 'Na4(NiO2)9_mp-882363.cif' NaNiF3_mp-1078237.cif NiF3_mp-561428.cif
H2O_mp-696735.cif 'K3(NiO2)2_mp-2740887.cif' KO2_mp-1866.cif Li2NiO2F_mp-1272313.cif LiH3O2_mp-625211.cif LiO8_mp-1235185.cif 'Na5(NiO2)6_mp-765679.cif' NaNiF3_mp-561480.cif NiF3_mp-614777.cif
H2O_mp-697111.cif 'K3(NiO2)2_mp-27565.cif' KO2_mp-2035026.cif Li2NiO2F_mp-1283454.cif LiHF2_mp-24199.cif LiO8_mp-1235252.cif 'Na5(NiO2)8_mp-765844.cif' NaNiO2_mp-1272149.cif NiH_mp-24719.cif
H2O_mp-703459.cif K3Ni2F7_mp-560449.cif KO2_mp-3346628.cif Li2NiO2F_mp-758524.cif LiHO_mp-23856.cif LiO8_mp-1236127.cif 'Na5(NiO2)9_mp-760267.cif' NaNiO2_mp-1274267.cif NiO_mp-19009.cif
H2_mp-1188177.cif 'K4(NiO2)3_mp-1104174.cif' K_mp-10157.cif Li2NiO2_mp-19308.cif LiHO_mp-625998.cif Li_mp-10173.cif Na5NiHO4_mp-759009.cif NaNiO2_mp-1274483.cif Ni_mp-23.cif
H2_mp-24504.cif K9Ni2O7_mp-13749.cif K_mp-1184755.cif Li2NiO3_mp-556550.cif LiH_mp-23703.cif Li_mp-1018134.cif Na5NiO4_mp-21996.cif NaNiO2_mp-1279798.cif O2_mp-1009490.cif
H2_mp-2739136.cif KF2_mp-976802.cif K_mp-1184764.cif Li2NiO3_mp-674420.cif LiNi2O3_mp-1639253.cif Li_mp-1063005.cif Na6(NiO2)7_mp-850287.cif NaNiO2_mp-19149.cif O2_mp-1087546.cif
H2_mp-632172.cif KF3_mp-1544557.cif K_mp-1184804.cif Li2O2_mp-841.cif LiNi2O3_mp-1644676.cif Li_mp-135.cif Na6NiO4_mp-1569694.cif NaNiO2_mp-578611.cif O2_mp-12957.cif
H2_mp-632291.cif KF3_mp-2749823.cif K_mp-1184808.cif Li2O_mp-1960.cif LiNi2O3_mp-757063.cif Li_mp-51.cif Na6NiO4_mp-779898.cif NaO2_mp-1545216.cif O2_mp-1524462.cif
H2_mp-730101.cif KF3_mp-867934.cif K_mp-1185201.cif 'Li3(NiO2)4_mp-1045574.cif' LiNi3O4_mp-1273274.cif Li_mp-567337.cif 'Na7(NiO2)10_mp-760203.cif' NaO2_mp-1901.cif O2_mp-2204849.cif
H2_mp-731827.cif KF_mp-463.cif K_mp-1545455.cif 'Li3(NiO2)4_mp-1313788.cif' LiNi3O4_mp-1275948.cif Li_mp-976411.cif 'Na8(NiO2)9_mp-760204.cif' Na_mp-10172.cif O2_mp-2739215.cif
H2_mp-738409.cif KH3F4_mp-29331.cif K_mp-2739257.cif 'Li3(NiO2)4_mp-754896.cif' LiNi3O4_mp-2760269.cif 'Na(NiO2)2_mp-1176434.cif' Na9Ni11020_mp-760849.cif Na_mp-1186081.cif O2_mp-610917.cif
H2_mp-850274.cif KH3O2_mp-28263.cif K_mp-58.cif 'Li3(NiO2)4_mp-755972.cif' LiNi3O4_mp-755956.cif 'Na(NiO2)2_mp-2750663.cif' NaF_mp-682.cif Na_mp-127.cif O2_mp-611836.cif
H2_mp-973783.cif KH4O2F_mp-983327.cif K_mp-604318.cif Li3Ni508_mp-2767662.cif LiNi405_mp-677318.cif 'Na(NiO2)2_mp-764934.cif' NaH15O8_mp-1201186.cif Na_mp-1525464.cif O2_mp-723285.cif
H3F2_mp-1184796.cif KH5O3_mp-2761095.cif K_mp-972981.cif Li3Ni508_mp-756159.cif LiNi607_mp-753344.cif Na14Ni2O9_mp-764496.cif NaH3O2_mp-24193.cif Na_mp-1545923.cif OF2_mp-1095223.cif
H3F2_mp-1524481.cif KH5O3_mp-676232.cif 'Li(NiO2)2_mp-1172967.cif' Li3Ni508_mp-758143.cif LiNiF3_mp-758501.cif Na2(NiO2)5_mp-760161.cif NaH3O2_mp-625391.cif Na_mp-2018774.cif
H3O_f_mp-27714.cif KH8O4F_mp-707068.cif 'Li(NiO2)2_mp-1314210.cif' 'Li4(NiO2)5_mp-763578.cif' LiNiH2_mp-1147649.cif Na2H16O9_mp-505185.cif NaH8O5_mp-733637.cif Na_mp-973198.cif
H4OF2_mp-23798.cif KH9O5_mp-28196.cif 'Li(NiO2)2_mp-504102.cif' Li4Ni509_mp-766892.cif LiNiO2_mp-1176588.cif Na2HF4_mp-37458.cif NaH9O5_mp-3346528.cif Na_mp-974558.cif
H6OF4_mp-28003.cif KHf2_mp-23846.cif 'Li(NiO2)2_mp-774941.cif' Li4Ni7011_mp-768091.cif LiNiO2_mp-2348641.cif 'Na2Li(NiO2)3_mp-1290445.cif' NaH9O5_mp-3347018.cif Na_mp-974920.cif
```

Last training epoch:

```
Epoch 100/100
405/405  225s 555ms/step - categorical_accuracy: 0.9739 - loss: 0.0794 - val_categorical_accuracy: 0.9
488 - val_loss: 0.3135
127/127  12s 91ms/step - categorical_accuracy: 0.9417 - loss: 3.9597
Test Accuracy: 94.1728413105011%
```

Test on Li-rich NMC (lab sample)

Filename: LNO1_A.xy



T

h

x

