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## Context & core issue

## Fig. 1 — Local magnetisation & deformation

## Fig. 2 — DFT energy, pressure & deformation

Fixed DFT hyperparameters  
across full database

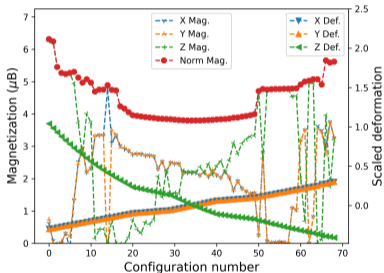
Undetected magnetic  
ordering transition

Corrupted  $E, F, \sigma$   
in training set

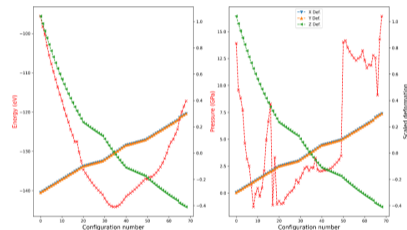
MLIP blind to  
magnetic state

## Poster content

- Quantification of data corruption
- Diagnostic workflow
- Magnetically-aware training strategies [WIP]



The magnetisation norm (red dots) jumps abruptly near configs. 15 and 50, marking AFM3k  $\rightarrow$  AFM2k and AFM2k  $\rightarrow$  AFM1k transitions. Simultaneous reordering of X/Y/Z components confirms a spin-structure change, not a numerical artefact.



Left: DFT energy (red) and lattice deformation. Right: DFT pressure (red) spikes at configs. 15 and 50, coinciding exactly with the magnetisation jumps in Fig. 1. An MLIP without magnetic labels cannot disentangle magnetic from structural contributions.

## Consequence

Similar structures carry different  $E/F/\sigma$  depending on the hidden magnetic state  $\Rightarrow$  systematic training-data inconsistency.