I. SYMMETRY CHANGES DURING SYMMETRY CONSTRAINED RELAXATIONS

Carrying out a symmetry constrained relaxation in VASP prevents symmetry breaking, but in some instances, we can see the merger of distinct Wyckoff positions into higher symmetry Wyckoff positions. This can lead to a change in the Wyckoff representation in screening workflows between the pre-relation and relaxed structures. To ensure that we have a well-defined map, we train Wren models to learn the target properties as a function of the relaxed Wyckoff representation.

A change in Wyckoff representation was observed in 29,417 out of 257,486 materials in the WBM data set. Consequently, the Wyckoff representation appears to change during relaxation for approximately 10% of candidates produced using prototype-based substitution workflows.

II. ENRICHMENT AS A FUNCTION OF DISTANCE TO THE CONVEX HULL

Figure S1 shows a stacked histogram of the energy to the convex hull of the full MP data set for the materials from the WBM data set. The histogram sections are coloured according to whether the Wren model correctly predicts a candidate to be below the known convex hull given its Wyckoff representation.

III. EXTRAPOLATION IN MATERIAL SPACE

The WBM data set was generated using an iterative workflow where successful candidates from the first batch were included when generating candidates for the second batch. As a consequence, candidates considered in later batches are likely to be less similar to materials contained in the MP data set. We use this stratification to probe how Wren’s performance changes as it is asked to make larger and larger extrapolations. We can make use of this stratification to

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**Figure S1.** Wren efficiently identifies stable structures when screening diverse chemical spaces. Histogram of the energy to the convex hull for materials in the WBM data set. The histogram is broken down into true positives, false negatives, false positives, and true negatives based on whether the Wren model predicts candidates to be below the known convex hull. Wren exhibits a high recall with the majority of materials below the convex hull being correctly identified by the model.

**Figure S2.** Rolling MAE of the Wren model on the WBM data set batches. Rolling mean absolute error of Wren on the batches of the WBM data set as the energy to the convex hull is varied. We take the pre-relaxation WBM Wyckoff representation as input. A windowing period of 40 meV per atom is used when calculating the rolling average. The curves show that later batches, believed to be more likely to be chemically dissimilar to the training data, incur higher average errors.
probe how Wren’s performance changes as it is asked to make larger and larger extrapolations by looking at how the mean absolute error changes as a function of the distance from the convex hull for the different batches. In Figure S2 we see that, whilst the overall shape of the curves remains the same as the V-shape seen for the full data set, there is an offset between the batches with later batches incurring higher errors on average.

IV. TAATA DATA SET DETAILS

The TAATA data set was originally constructed in [35] using an exhaustive prototyping strategy. Initial prototypes were extracted from the Inorganic Crystal Structure Database (ICSD) and the Crystallography Open Database (COD). All inequivalent structures with one anion and two cations containing less that 41 atoms were used. In total, 2,444 structures satisfied these criteria and were used for prototyping. In each case the anion was replaced by N, and the cations were substituted with one of the \{Ti, Zr, Hf\} species and Zn. Both permutations of \{Ti, Zr, Hf\} species and Zn were considered. The starting volume of each structure was rescaled to give the same atom to unit cell ratio as in the ground state structures. In addition to ternary, binary, and elemental structures from the Materials Project database were also included in the search.

V. PHASE DIAGRAM CONSTRUCTION

Figure S3 shows phase diagrams constructed from the initial Wren predictions as well as the nominal ground truth phase diagram when all the DFT calculated energies are considered. In order to demonstrate that Wren aids our exploration of unexplored systems we also show the resulting phase diagrams after 300, 800 and 1,300 calculations have been carried out after triaging calculations using the predicted energy above the convex hull constructed using the predictions of the Wren model. These intermediary plots show that whilst superficially the zero-shot hulls generated by Wren do not match the DFT computed hulls using the Wren predictions to triage calculations gives phase diagrams that closely resemble the exhaustive DFT computed phase diagram, each missing just a single stable phase, after just 300 calculations.

In the manuscript we choose to look at how well the approach performs on selecting candidates within 10, 20 and 30 meV per atom of the DFT computed convex hull in order to collect more reliable statistics. If we focus on just the DFT computed stable phases, we see that our model does rank a stable phase outside the top 300 in each of the systems studied. Checking these erroneous predictions reveals that they are all structures for which no isopointal analogues exist in the training data. It is worth noting that the fact TAATA considers three group 4 elements, \{Ti, Zr, Hf\}, makes the prediction task significantly more challenging as we have no prior tertiary examples that share the same group chemistry.

VI. LEARNING EFFICIENCY

Applications in material science, particularly the investigation of functional properties of materials, often encounter issues with data scarcity. Given this, the learning efficiencies of models used in material science applications are of critical importance. The best way to probe this is through the construction of learning curves [40-41]. A learning curve depicts the error of a model on a fixed test set as the amount of data used to train the model is varied. We see in Figure S4 that both individual Wren models and Deep Ensembles of Wren models follow unbroken power law relationships. Consequently, we would expect that as more data is obtained the accuracy of the proposed model should continue to improve.

VII. ALTERNATIVE STRUCTURE-BASED MODELS FOR MATERIALS DISCOVERY

To contextualise the performance of the Wren model, we compare against CGCNN, a well-established message passing neural network for predicting the properties of inorganic materials based on the “crystal-graph” of local atomic environments [20], and a baseline consisting of a Random Forest [70] paired with the Voronoi crystal structure attributes [71] plus Magpie composition descriptors [7] as proposed in [71] that we refer to as the Voronoi model.

In prototype-based substitution workflows, such as that used to generate the WBM data set [16], the distributions of bond distances seen before relaxation can be highly unphysical as the original species often have very different atomic radii to the substituted species. Consequently, models such as CGCNN that directly encode local environments based on bond distances are likely to suffer from significant degradation in performance when moving from screening relaxed crystal structures to screening pre-relaxation crystal structures [22]. The Voronoi crystal structure attributes are constructed conceptually distinct manner, using the areas of the Voronoi facets around a given site to weigh local property differences between sites in such a way that the resulting features are invariant to changes in volume. This is a compelling property as one of the principal changes that occurs when relaxing a prototype structure after chemical substitution is the change in the unit cell volume.

As expected, we see that using CGCNN to predict the stability of candidate materials based on their relaxed structures is highly accurate. However, as previously noted, in prospective workflows we do not have access to relaxed crystal structures. When we compare the stability predictions obtained when using CGCNN to estimate the stability of candidate materials based on their pre-relaxation structures, we see a substantial degradation in performance in keeping with the results of prior works [22].
Figure S3. Phase Diagrams for the TAATA Data Set as Wren is used to Triage Calculations. Whilst
the zero-shot phase diagrams generated by the Wren model do not appear visually similar to the DFT computed phase
diagram, we see that using the energy above the hull to the zero-shot convex hull is an effective surrogate for stability.
Using this prediction to triage candidates allows for phase diagrams that closely resemble the DFT computed phase
diagrams to be constructed with as little as 300 calculations.

Figure S4. Learning curve for the Wren model with increasing training data. Learning curves for
both single and Deep Ensembles of Wren models shown on log-log scales. The curves are produced by plotting the
error on a fixed test set (here 5% of the union of the MP and WBM data sets) as the amount of data used to train
the model is increased. A grey guideline shows the size of the test set. The learning curve shows that a power-law
relationship exists between the amount of training data and the MAE of the trained model.

Turning to the Voronoi model, we see that robustness of the Voronoi crystal structure attributes is confirmed in the observation that the relaxed and pre-relaxation structures make similar predictions on the WBM data set after having been trained on the MP

Figure S5. Comparison of Errors of Wren, Voronoi, and CGCNN Models on WBM with Distance to
the MP Convex Hull. Figure replicates experimental setup of Figure 2 comparing the Voronoi model against
CGCNN and Wren. A scale bar is shown for the windowing period of 40 meV per atom used when calculating the rolling average. Grey guidelines highlight 100 meV per atom, 50 meV per atom and the MAE = |ΔE_{Hull-MP}|. The Wren model is more accurate than both the Voronoi model and CGCNN on pre-relaxation structures but, as expected, it is less accurate than CGCNN on relaxed structures. Wren is more accurate than the Voronoi model on relaxed structures highlighting the strengths of Wren and the Wyckoff representation.
Figure S6. Variation in Precision and Recall for Wren, Voronoi, and CGCNN Models with Calculation Count. Precision and Recall on the WBM data set for Wren, Voronoi, and CGCNN as the number of calculations increased. The precision is shown with a dashed line and the recall is shown with a dotted line. Crosses are used to mark the termination points where the models no longer believe there are anymore materials in the WBM data set below the MP convex hull. Initially both Voronoi and CGCNN models have much lower precision than Wren. However the precision of CGCNN plateaus and then is upper-bounded by that of the Wren model until it terminates with a recall of 61%. The Voronoi model has much lower precision and terminates with a recall of 55% after ~ 77,000 calculations.

data set (see Figure S5). Quantitatively a mean absolute deviation of 19 meV per atom between the pre-relaxation and relaxed structure predictions is seen for the Voronoi model with is small compared to the MAEs of 145 and 142 eV per atom respectively. Despite this robustness, the Voronoi model results in a much larger error than Wren.

We note that even though screening for stability using the pre-relaxation structures is not very accurate, using structure-based models in this manner still leads to enrichment in virtual screening workflows, for example, Park et al. have used this approach alongside their “improved”-CGCNN model [22] to accelerate the discovery of novel stable compounds within the ThCr$_2$Si$_2$ structure-type achieving a precision of 13%. Whilst such workflows offer an improvement over conventional screening workflows in terms of enrichment, the limited accuracy of using structure-based models in this manner leads to low recall – the Voronoi model achieves a recall of 55% and the CGCNN model achieves a recall of 61% of the materials in the WBM data set below the known convex hull compared to a recall of 76% for Wren (see Figure S6).

Accordingly, several attempts have been made to improve the performance of structure-based models when making stability predictions on pre-relaxation structures but attempting to make models that are robust to changes that occur during structure relaxation. The symmetry-labelled Voronoi graph convolutional neural network of [72] tries to do this by discarding explicit distance information. Instead, edges in the graph are labelled by the approximate symmetry of the Voronoi facets. This leads to a smaller deterioration in accuracy than seen for distance-based models. More recently, the BOWSR algorithm [73] has been introduced to directly minimise the domain shift between pre-relaxation and relaxed structures using a surrogate model. The algorithm uses Bayesian optimisation to adjust the free parameters of pre-relaxation symmetrised structures according to a trained structure-based energy model. This process yields pseudo-relaxed structures and results in smaller errors in materials discovery tasks.
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