

## STRUCTURE GENERATION



## CANDIDATE SPACE

### 1. CANDIDATE SELECTION

Exploration of the predicted space for searching new structures using an acquisition function



### 5. PREDICTIONS

Formation energy estimates and uncertainty of the model of “unseen” atomic structures.



## ACTIVE LEARNING

### 2. FIRST-PRINCIPLES CALCULATIONS

Performing atomic-scale simulations using quantum mechanics



### 4. MACHINE LEARNING MODELS

Building machine learning models training and testing for atomistic structures and their properties.



### 3. FEATURE ENGINEERING

Extracting and selecting features from the computed atomic structures

