

# Computational Design of Materials via Convolutional Neural Networks

E. Tomy George, J. A. Muñoz and O. Fuentes

November 6<sup>th</sup>, 2021

The phase diagram is a type of chart used to show the conditions at which thermodynamically distinct phases occur and coexist at equilibrium. In the case of alloys, these phases include the liquid stage and the different solid crystal structures that the alloy can be found depending on the temperature and percentage mixture of each metal. Determining a phase diagram is done experimentally, which is extremely expensive. We propose using a machine learning model to obtain phase diagrams. We plan to use convolutional neural networks (CNN) trained on the displacement of atoms of the alloy from their equilibrium positions in a crystal to predict the potential energy of the alloy, from which the phase diagram can be obtained. CNNs were chosen since they are space-equivariant. The alloy of Copper (Cu) and Silver (Ag) will be used to train the CNN model, since the Cu-Ag phase diagram is readily available, serving as a comparison for the CNN's predictions.