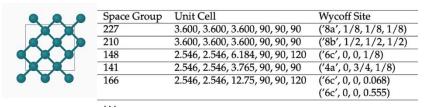
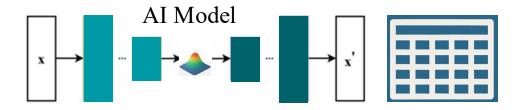
(a) The LEGO-XTAL Framework

Step 1: Data Augmentation & Tabularization

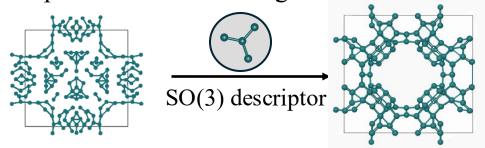




Step 2: Featurization, Training & Sampling



Step 3: Relaxation to Targeted Environment



Step 4: Energy Ranking (MACE/VASP)

(b) Application to sp² carbon

