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Connecting Molecular Dynamics to Experiment using Machine Learning[1] PARKER HAMILTON, Brigham Young University, REMI DINGREVILLE, Sandia National Labs — Current resources allow for investigation of large parameter spaces of materials and material properties or processes using atomistic simulations much more quickly than by experiment. An additional advantage to simulation is the level of detail available in the results, namely atom positions, which can be difficult to recover from experimental results. We propose a process to connect experimental images, such as STEM, with similar atomistic simulation results; focusing specifically on defect crystal structures.

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