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Grain Boundary Representation and Property Prediction[1] J. SPENDLOVE, Brigham Young University, E. HOMER, L. SERAPHIN, G. HART, BYU — A grain boundary (GB) is the interface between distinct crystals (or grains) of a solid, crystalline structure. The type and frequency of these GBs in a material can exert significant influence on macroscopic material properties including strength, thermal conductivity, hydrogen embrittlement and corrosion resistance; however, much is still unknown about these connections. Our aim is to develop and use expressive, smoothly varying atomic descriptions of GB structure to enable effective machine learning property prediction. One of the most promising atomic models that enables GB structure representation is the Smooth Overlap of Atomic Positions descriptor, or SOAP, which utilizes Gaussian density distributions and spherical harmonics. The SOAP characterization can be processed into two descriptors that have been developed by our group to enable machine learning: the Averaged SOAP Representation (ASR) and the Local Environment Representation (LER). In previous works, machine learning using both ASR and LER have been shown to successfully predict material properties based on GB structure. This presentation focuses on these methodologies, their integration into the Python-based scientific code `pyrelate`, and their effect on the quality of machine learning.

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