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Using Machine Learning to Accelerate Complex Atomic Structure Elucidation WILLIAM BROUWER, LAZARO CALDERIN, JORGE SOFO, The Pennsylvania State University — Workers in various scientific disciplines seek to develop chemical models for extended and molecular systems. The modeling process revolves around the gradual refinement of model assumptions, through comparison of experimental and computational results. Solid state Nuclear Magnetic Resonance (NMR) is one such experimental technique, providing great insight into chemical order over Angstrom length scales. However, interpretation of spectra for complex materials is difficult, often requiring intensive simulations. Similarly, working forward from the model in order to produce experimental quantities via ab initio is computationally demanding. The work involved in these two significant steps, compounded by the need to iterate back and forth, drastically slows the discovery process for new materials. There is thus great motivation for the derivation of structural models directly from complex experimental data, the subject of this work. Using solid state NMR experimental datasets, in conjunction with ab initio calculations of measurable NMR parameters, a network of machine learning kernels are trained to rapidly yield structural details, on the basis of input NMR spectra. Results for an environmentally relevant material will be presented, and directions for future work.

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