1171-65-221 **Barry C Husowitz*** (husowitzb@wit.edu), 550 Huntington Ave., Boston, MA 02115. *Artificial Neural Networks (ANN) Applied to Monte Carlo and Molecular Dynamic Simulations.* Preliminary report.

The computational expense to accurately simulate large atomistic systems is enormous. In order to overcome this computational cost empirical potentials are used, which rely on parameters that are adjusted to reproduce either experimental or first principle references. Furthermore, careful parameterization of such potentials can be challenging and must be validated for each system. Artificial Neural Networks (ANN) approaches such as those proposed by Behler and Parrinello circumvent this parameterization problem by employing machine learning techniques to calculate the potentials. The Behler-Parrinello approach calculates the potential energy surface based off a set of reference calculations. This approach has the advantage that it can be well automated, new potentials can be constructed easily, permits application of potentials to arbitrary structures, and reaches accuracies comparable to first principle methods with a much lower computational cost. I am interested in using ANN's to calculate potential energy surfaces to use in Monte Carlo simulations and Molecular dynamic simulations of crystal structures. In particular, I am interested in simulating the crystal structure of Perovskite to obtain x-ray scattering data that we can compare to experimental results. (Received August 16, 2021)