Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Studies of Glass vs Crystal Forming Abilities and other Far-From-Equilibrium Phenomena Using Machine Learning WADE FUERSTE, YANG ZHANG, Univ of Illinois - Urbana — Far-from-equilibrium reactions and processes have been long known to exist, but the quantitative understanding of these phenomena have been challenging. This is partly due to their diverse range of timescales that are occurring out of the range of existing methods. Previous attempts to quantify this area of research have fallen short due the large computational costs or accurate measurements at the molecular level over second, and larger, timescales. Our group exploits a range of non-equilibrium processes all containing large scale fluctuations and heterogeneity. We aim to develop and apply machine learning algorithms, built upon molecular simulations, to sample statistically rare events efficiently and understand the long timescale phenomena from the molecular level. With machine learning we analyzed large sets of data, beyond standard computational means, to gain a more accurate understanding of these far-from-equilibrium processes. Herein, we will show new insights provided by machine learning analysis on the dynamics of supercooled liquids and glasses, nucleation and crystal growth rates.

Wade Fuerste
Univ of Illinois - Urbana

Date submitted: 06 Jan 2017 Electronic form version 1.4