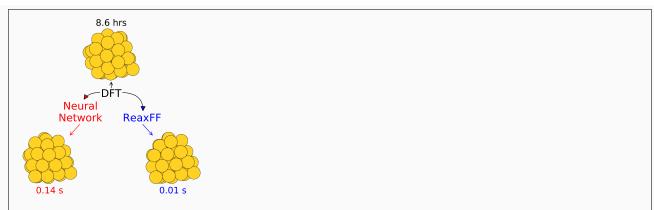# Graphical Abstract

January 18, 2016

Predicted minimum energy structures for 38 atom Au cluster from a total of 125 configurations for KS-DFT, Neural Networks, and ReaxFF. Calculation times are also shown for comparison.