## Abstract

This paper describes an object-oriented Python programming project designed to perform simulated annealing Monte Carlo simulations of molecular clusters and thereby find the lowest energy geometry of each cluster. Clusters studied include homogeneous systems consisting of a single species and heterogeneous systems consisting of multiple species. Example studies were performed on water clusters $[(\mathrm{H2O})_n, n = 2, \ldots, 5]$ and clusters of ammonium chloride $[(\mathrm{NH_4Cl})_n, n = 1, 2 \text{ and } 4]$. Simulations are performed using mag-walking to ensure ergodic sampling and molecules are treated as rigid bodies. A comparison with previous studies shows that the cluster geometries and conformer energies obtained from the program agree well with literature values. This project will ultimately result in the public release of the first simulated annealing Monte Carlo program which includes mag-walking.