Abstract Submitted
for the TSF16 Meeting of
The American Physical Society

An Empirical Three-Body Potential for Tetrahedral Liquids
JOSHUA AMBURGEY, JACOB URQUIDI, GREGGORY MCPHERSON, New Mexico State University, X-RAY AND NEUTRON SCIENCE LABORATORY TEAM — A simple three-body empirical potential function is proposed for computational studies of liquid water and other liquids possessing tetrahedral coordination. The potential is derived from a linear combination of nearly degenerate structural forms. The potential presented has three types of minima associated with the structure of liquid water; one nearest neighbor and two next-nearest-neighbor minima. The inner minima corresponds to the hydrogen bonded distance of 2.78Å present in liquid water whilst the other two minima represent the non-hydrogen bonded neighbor normally present at a tetrahedral distance of 4.5Å but which begins to occupy an interstitial distance of 3.4Å with increased pressure, increased temperature, increased confinement, and changes in pH. The 3.4Å distance is populated at the expense of the 4.5Å distance and it is these two explicit bonding distances in the liquid which gives rise to the anomalous behavior of liquid water.

Joshua Amburgey
New Mexico State University

Date submitted: 26 Sep 2016 Electronic form version 1.4