Sandia National Laboratories

Reese Jones
P. O. Box 969,
Sandia National Laboratories,
Livermore, CA 94551-0969, USA
(925) 294-4744
rjones@sandia.gov

The Journal of Chemical Theory and Computation

May 21, 2015

Dear Editors,

We would like to submit our manuscript "Efficient use of *ab initio* calculations to generate accurate Newtonian dynamics " for publication in the *The Journal of Chemical Theory and Computation* as a article. In the paper we develop a new method of using *ab initio* calculations to drive classical dynamics that has the potential to scale to system sizes approaching those feasible with traditional empirical molecular dynamics. The method relies on a database of pre-computed Hellmann-Feynman forces associated with local atomic configurations. Using a distance metric on these configurations we are able to do fast searches through the database for similar configurations and also to form a local interpolation of the stored forces at configurations generated by the dynamics. This pairing of configurations and forces supplants the traditional globally fitted empirical potential. The approach is shown to be convergent and have acceptable accuracy and conservation properties. All details necessary to apply the method are given.

Sincerely,

Reese Jones and Mickey Shaughnessy