Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

An Efficient Real-Space Implementation of the van der Waals Energy and Analytical Forces in Plane-Wave Ab Initio Molecular Dynamics
ROBERT DISTASIO, ZHAOFENG LI, ULRICH ASCHAUER, Princeton University, XIFAN WU, Temple University, ROBERTO CAR, Princeton University — In this work, we present an efficient algorithmic implementation of the energy and analytical forces of the recent density functional based van der Waals (vdW) correction proposed by Tkatchenko and Scheffler (PRL 102, 073005 (2009)) within the framework of plane-wave based ab initio molecular dynamics. The algorithm presented herein is a highly parallelizable, order (N) formulation that allows for accurate treatment of large molecular systems with a computational cost that is negligible with respect to the underlying evaluation of the exchange-correlation functional. The computational resources and performance of our algorithm, which utilizes a real-space implementation of the molecular pro-density, will be analyzed and compared against a reciprocal-space formulation of the Hirshfeld volume based on a spherical wave expansion of the underlying plane-wave basis. The effects of this vdW correction are demonstrated within the context of the oxygen-oxygen and oxygen-hydrogen radial distribution functions obtained via highly accurate PBE0-based liquid water simulations.

Robert DiStasio
Princeton University

Date submitted: 19 Nov 2010 Electronic form version 1.4