Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A van der Waals DFT Approach to Modeling Water[1] BRIAN KOLB, TIMO THONHAUSER, Wake Forest University — We present density functional theory calculations for small water clusters and bulk water including van der Waals interactions via the non-local functional vdW-DF [1]. Historically, standard functionals such as LDA or GGA have been unable to accurately predict vibrational frequencies of small water clusters or the freezing point of bulk water, which has been partly attributed to the lack of van der Waals interactions [2]. We have implemented vdW-DF in the PWscf package, using an efficient convolution approach [3]. Our results for the vibrational frequencies of small water clusters show that vdW-DF gives a significant improvement compared to LDA or GGA. While the discrepancy between experiment and LDA/GGA is as much as 28% for certain modes, vdW-DF reduces this error to only about 6%. We also present results for the vibrational spectrum and Raman spectrum of periodic ice, again showing the advantages of vdW-DF. In addition, we show preliminary results for bulk water from our vdW-DF MD simulations.

[1] Thonhauser et al., Phys. Rev. B **76**, 125112 (2007).
[2] H. Sit and N. Marzari, J. Chem. Phys. **122**, 204510 (2005).
[3] G. Roman-Perez and J. Soler, Phys. Rev. Lett. **103**, 096102 (2009).

[1]We acknowledge support from ORAU.

Brian Kolb
Wake Forest University

Date submitted: 16 Nov 2009 Electronic form version 1.4