

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

A Density Functional Theory Study of the Non-local Correlations between Nucleic Acid Base Pairs VALENTINO R. COOPER, TIMOTHONHAUSER, DAVID C. LANGRETH, Rutgers University — The interactions of nucleic acid bases are fundamentally important in determining the behavior and structure of biologically important molecules such as DNA and RNA. However, the stacking of nucleic acid bases in a strand of genetic material involves significant van der Waals forces, which are often inaccurately represented or too expensive to compute in many modern theoretical methods. In this paper, we use Density Functional Theory (DFT) with a non-local van der Waals correlation functional¹ to study the stacking interactions of nucleic acid base pairs. This method correctly and seamlessly accounts for the long-range interactions present among isolated fragments through a density-density interaction formula. Since this technique is implemented within DFT it has the advantage of being able to draw on the speed, efficiency and accuracy of this *ab initio* method.

¹M. Dion, H. Rydberg, E. Schröder, D. C. Langreth and B. I. Lundqvist, Phys. Rev. Lett. **92**, 24601-1 (2004).

Valentino R. Cooper
Rutgers University

Date submitted: 29 Nov 2005

Electronic form version 1.4