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**Density Functional Analysis of Stabilizing Effects of Stacking Interactions in Nucleic Acid Base Pair Steps** DAVID C. LANGRETH, VALENTINO R. COOPER, TIMO THONHAUSER, AARON PUZDER, Rutgers University, ELSEBETH SCHRÖDER, BENGT I. LUNDQVIST, Chalmers University of Technology — Base pair stacking interactions contribute significantly to the stability of DNA. In addition, numerous studies highlight the stabilizing effect of thymine within DNA. Electrostatic, van der Waals (vdW) and hydrophobic interactions all contribute to these stacking interactions, but their relative contributions are unclear. In this paper, we use the newly developed vdW density functional[1] to investigate the importance of vdW interactions to stacking interactions between Watson-Crick DNA base pairs. Our results indicate that these interactions are essential for defining both the base pair step distance and the helical twist angle of DNA. Furthermore, we show that the stability gained from the presence of thymine is due to vdW interactions between the methyl group of the thymine with neighboring bases.

[1]Dion, Rydberg, Schröder, Langreth, Lundqvist, PRL **92**, 246401 (2004)

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