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Theoretical investigation of using armchair and zigzag carbon nano rings for DNA sequencing based on density functional theory

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Abstract

Based on density functional theory (DFT) at the B3LYP level, we investigated the interaction of DNA nucleobases with carbon nano-rings in armchair and zigzag shapes. Van der Waals correction was applied to describe the long range term of bipolar interaction. Results indicate that a net electric charge was not transferred between the DNA bases and the carbon nano-rings. This indicates the interaction is of physical type. Outcomes show the following order for the strength of the interaction between the carbon nano-ring (9,9) and the four DNA nucleobases: guanine > adenine > cytosine > thymine. The corresponding order for the zigzag carbon nano-ring (15.0) is adenine ≈ guanine > cytosine > thymine, suggesting carbon nano-ring (9,9) may have a potential to specify the sequencing of DNA.

Keywords: DNA sequencing, carbon nano ring, density functional theory, binding energy, Van-der-Waals correction

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