DNA Electronic Circular Dichroism Spectra at the Inter-Base Pair Scale

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DNA is the central molecule of life. While it is mainly known for its storage of genetic information, DNA is also involved in a myriad of molecular recognition events and activities of DNA-protein complexes and is capable of maintaining its supramolecular structures. These functions may be significantly affected by slight structural modifications of DNA, and the development of tools to predict its conformation is thus crucial to understand DNA biochemical processes.

Over the past years, circular dichroism (CD) has been widely used to elucidate the several conformations of DNA in solution (e.g., A-, B-DNA or G-quadruplexes).[1] Theoretical CD calculations are relevant to rationalize and forecast DNA chirality at the nanoscale. However, computational cost appears as a bottleneck for calculating the entire DNA CD-spectra regarding the size of the system. This may be bypassed by using a building-block approach based on base-pair dimers, i.e., by evaluating and summing two-body ECD contributions between direct neighbours. By reducing an entire double strand (ds) DNA to multiple base-pairs, each ECD two-body contribution can then be calculated using the complex polarization propagator (CPP) approach[3] in conjunction with DFT. This is successfully applied here to rationalize the ECD spectra of B-DNA dsDNA (dA)20(dT)20 case study as well as a nucleosomal DNA.[4]

References

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