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Lighting Up Non-Canonical DNA: Theoretical Insights into Photodriven Mechanisms

Since the 80s, when Ned Seeman [1] first envisioned the idea of building artificial structures using DNA, the field of DNA nanotechnology [2] has grown exponentially, especially due to the potential of combining light and DNA in applications beneficial to humans, such as phototherapy and optoelectronics. However, two main factors have limited its expansion: on one hand, canonical nucleobases do not exhibit optimal optical properties (such as fluorescence or energy transfer), and on the other, the theoretical description of such complex mechanisms in such large structures has been challenging.[3] With this aim in mind, we have characterized the main excited-state processes triggered by light absorption in non-canonical DNA structures. Specifically, we have modelled guanine quadruplexes (G4), both in solution and when interacting with photoswitches, as well as I-motifs and metallo-DNAs, using molecular dynamics and quantum chemical calculations.(4, 5) Interestingly, some of these structures exhibit behaviour distinct from that of canonical DNA strands, such as enhanced fluorescence or the charge-transfer mediated population of characteristic triplet excited states, boosting their potential biomedical or technological applications.

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