Intermolecular electron transfer in DNA damage and repair: insights from excited state calculations

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Redox properties of nucleobases are central in DNA damage by light and other agents and in enzymatic repair. Photoinduced interbase electron transfer leads to formation of asymmetric photoproducts between adjacent thymine bases such as 6-4 and spore photoproducts. Moreover, direct enzymatic repair of major photoproducts by DNA photoproduct lyases is ruled by forward and back electron transfer reactions. Contributions of the excited state calculations to the recent progress in these topics will be summarized. The focus will be on excited state calculations providing estimates of electron transfer rates. In the case of (6-4) photolyase, such calculations predict electron transfer rates in good agreement with those experimentally observed for the repair and futile electron transfer cycles. The impact of classical and quantum interactions of the active site system with its molecular environment will be highlighted.