

Modeling the dynamics of DNA (photo)lesions : from reactivity to repair.

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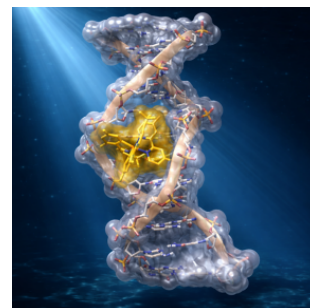
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Formation and repair of DNA lesions embrace a rich and combinatorial chemistry, where atomic-scale simulations are increasingly helpful to complement and extent experimental evidences.

The modeling of DNA structure, dynamics, and (photo)chemistry has benefited from a series of recent methodological developments that now allow, for instance capturing DNA-photosensitizers interactions, probing new excited-state mechanisms for DNA lesions induction or photostability [1], and rationalize the photochemistry or photocatalytic properties of drugs within DNA owing to hybrid QM/MM-MD schemes.



I will present a series of examples where computational approaches can palliate, at least partly, the absence of NMR, FRET or X-ray data for damaged DNA oligonucleotides, DNA-drug binding modes or even DNA-proteins interactions at the nucleosomal scale [2,3]. I will also situate DNA-ligand interactions, which can be helpful for the design of next-generation G-quadruplex-specific photosensitizers [4] or new DNA-inspired photocatalysts [5].

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