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Can low energy electrons lead to strand breaks in DNA under realistic conditions? JORGE KOHANOFF, MAEVE SMYTH, Queens University Belfast — It is widely accepted that low energy electrons produced by ionizing radiation play an important role in causing DNA damage [B. Boudaïffa et al., Science **287**, 1658 (2000)]. Understanding the behaviour of DNA components in the condensed phase due to such electrons is a fundamental step towards modelling this damage within a realistic environment. Here we present a computational study of the effect of low energy electrons in condensed phase models of solvated DNA fragments. First we show that excess electrons, which are initially found delocalized, quickly localize around the nucleobases within a 15 fs time scale. Energies and time scales are comparable for each of the bases [M. Smyth and J. Kohanoff, Phys. Rev. Lett. **106**, 238108 (2011)]. The phosphodiester bond $C_{3'}$-$O_{3'}$, which under normal conditions is very stable, weakens significantly upon electron attachment both, in the gas and in the condensed phase. Computation of free energy profiles show that barriers for bond cleavage are in the region of 5-8 kcal/mol for all the solvated nucleotides, thus suggesting that this kind of event is quite likely at ambient temperature. This supports the notion that ionizing radiation can actually lead to DNA strand breaks in the physiological environment.

Jorge Kohanoff
Queens University Belfast

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