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Modelling Proton Tunnelling in DNA Replication

Proton transfer between the DNA bases can lead to mutagenic Adenine-Thymine tautomers. In our work, we determine that the energy required for generating tautomers radically changes during the separation of double-stranded DNA. Our results demonstrate that the unwinding of DNA by a helicase enzyme could significantly enhance the stability of tautomeric base pairs and provide a feasible pathway for DNA spontaneous mutations. This image shows the site of such a double proton transfer in a A-T base pair within the nucleic acid duplex. To produce the image atomic coordinates were taken from molecular dynamics simulations (Gromacs on ARCHER2) before being rendered in VMD. A Van der Waals envelope was added to show the atoms used in quantum chemical models. The image has been further altered in Photoshop to highlight the delocalised nature of the tunnelling proton. The quantum chemical calculations were performed with NWChem on ARCHER2.

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