Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Stability of radiation-damaged DNA after multiple strand breaks

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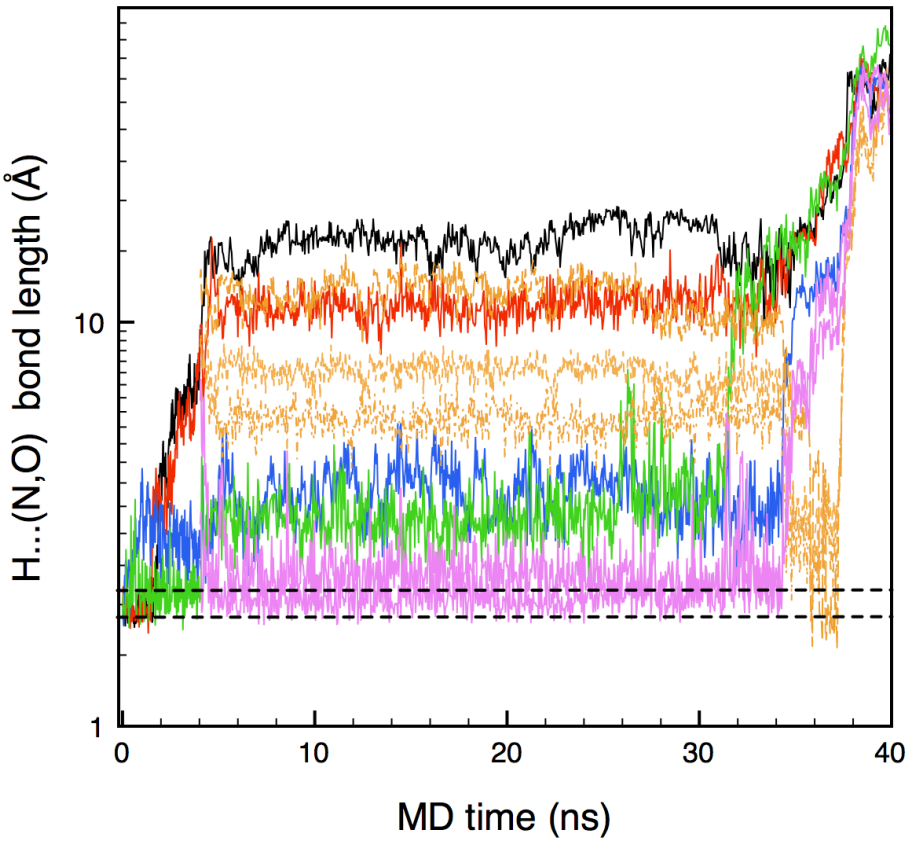
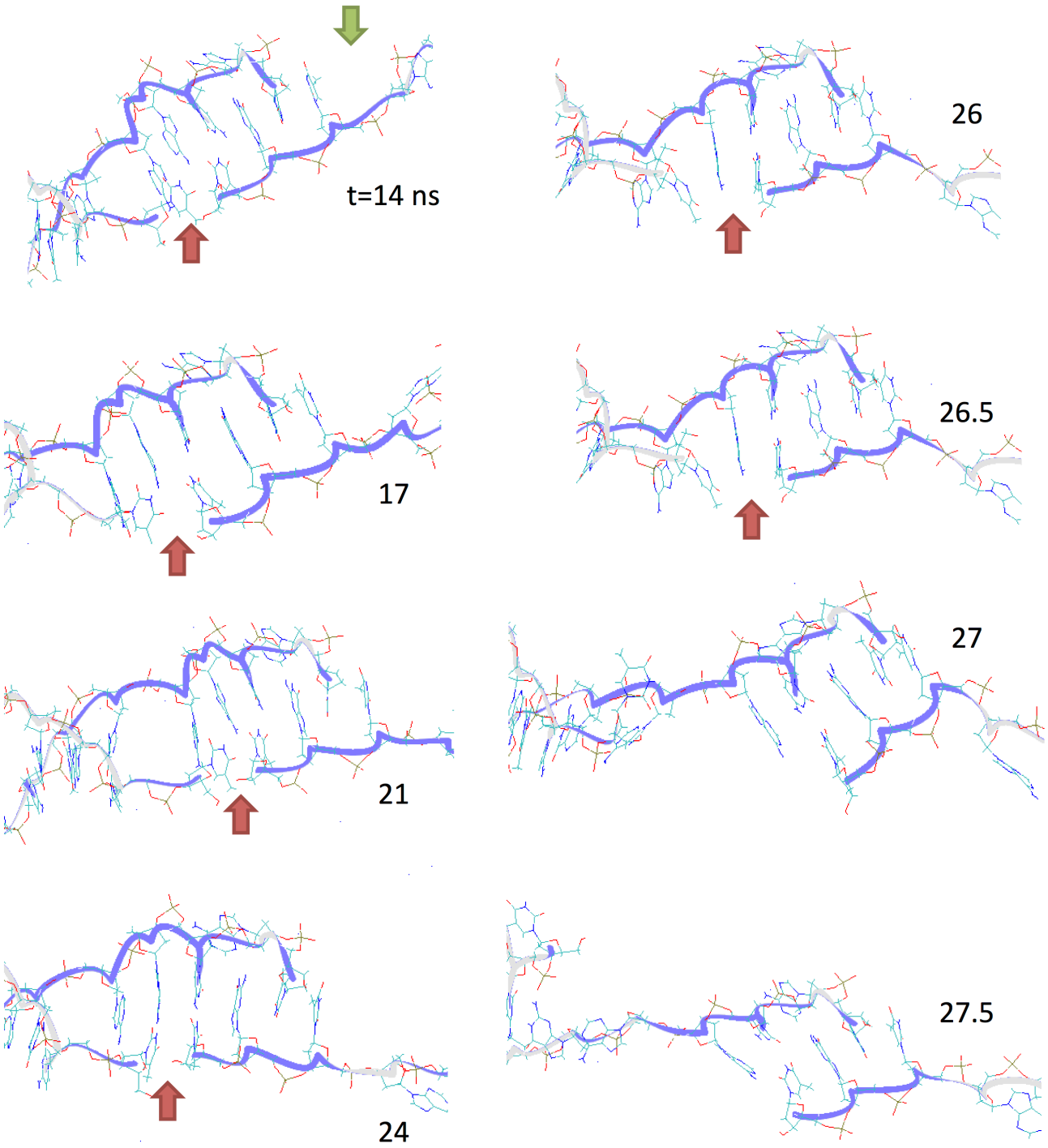
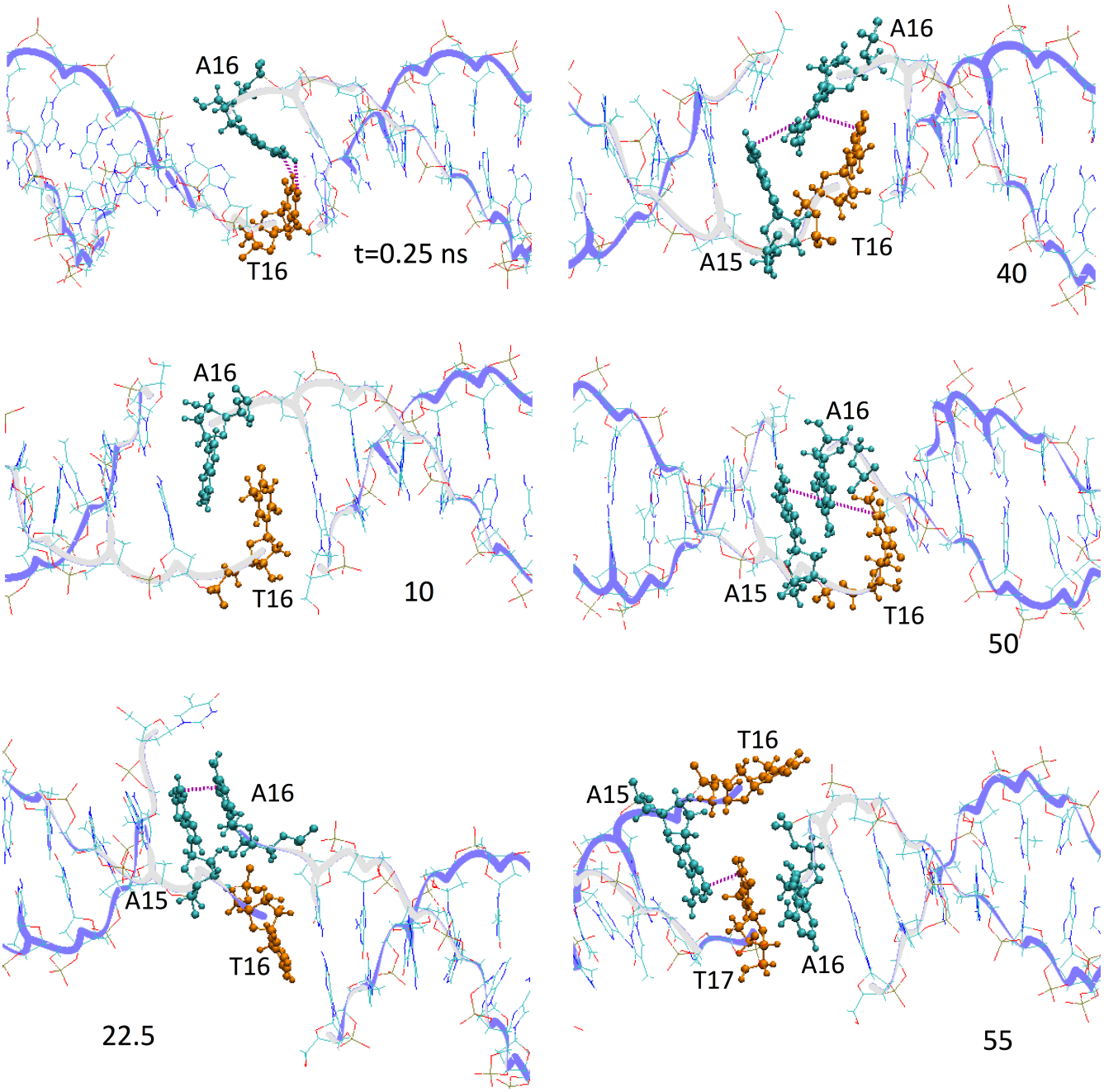
SUPPLEMENTARY MATERIAL



Supplementary figure 1 Plot of selected hydrogen-bond lengths (H-acceptor distance). Some H-bonds within the 4 base-pairs comprised between the backbone cuts of the DSB-4p configuration are shown, during a MD simulation at T=310 K, with spring constant 1,660 pN/nm, pulling velocity 4 cm/s. The two horizontal dashed lines delimit the H-bond length comprised between about 1.8 and 2.1 Å, large enough to cover thermal fluctuations. The first H-bonds to break, around t=0.4 ns (black), are identified as the G_{18}–C_{14} H...O bond; followed right after, between t ~1 and 2 ns (red), by both the H-bonds between T_{19}–A_{13}, the two bases being now split at one end of the DSB defect (see also the small peak of 40 pN at ~4% elongation in **Fig. 2b**). At the other end of the DSB, the (green) bonds between A_{16}–T_{16} still hold until about t=4.5 ns, when they split up. However, in the meantime new H...O and H...N bonds (pink) have formed, between the T_{19}–C_{14} and G_{18}–A_{15}, non-Watson-Crick base pairs. The last, short-lived H-bonds setting in right before the final DSB fracture (orange-dashed), between t=34 and 37 ns, are the "unusual" G_{18}–T_{16} H...O bonds, with the T oxygen belonging to the backbone.



Supplementary figure 2 Time sequence of eight snapshots of the DSB-4bp region from a SMD simulation at T=310K. The right-side strand break (green arrow) is already open before the first time-frame shown here, at *t* =14 ns. The left-side strand break (red arrow) is still closed, until the final opening occurring around *t* ~26 ns. After this time, the three bases of the lower strand continue to slide to the right with respect to the four bases of the upper strand, which slide to the left of the figure. The fourth base of the lower strand can be seen at the lower right corner, swinging back of the sugar-phosphate backbone, already from the early stages of the simulation.



Supplementary figure 3 Time sequence of six snapshots of the DSB-1bp, from a unconstrained-DNA thermal stability simulation at T=350K. The H-bonds between A_{16} and T_{16} are cleaved within 1 ns from the beginning. At *t*=10 ns, the two bases are seen in the new stacked configuration. At t=22.5, T_{16} has rotated by 180 deg about the backbone, and a new π-stacking interaction takes place between A_{16}–A_{15}. At *t*=40 ns, T_{16} has rotated back into place, but the DSB configuration is now quite distorted. At *t*=50 ns the DSB appears isolated from the rest of the DNA. At *t*=55 ns, immediately before the final DSB fracture, T_{16} and A_{16} are disconnected, and the residual A_{16}-T_{17} π-stacking interaction is the last one to be split apart.