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Title: Exploring destabilisation of DNA hairpins under nanoconfinement

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Abstract:

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Confinement in a DNA nanocavity is known to facilitate the stabilisation of Sec- ondary DNA structures such as G-quadruplexes and i-motifs. However, folding and unfolding experiments of duplex DNA hairpins in a nanocage indicate a decrease in the mechanical and thermodynamic stabilities. The dramatic reduction in the stabil- ities of confined DNA hairpins is primarily attributed to the reduced water activity in the DNA nanoassembly. We aim to explore this destabilisation's structural and thermodynamic aspects by modelling the DNA system and simulating the dynamic pulling using the coarse grain oxDNA model. We observe that the loss of conforma- tional space resulting from the constriction of the hairpin by the DNA nanocage does affect the mechanical and thermodynamic properties of the system.

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