DNA opening during transcription initiation by human RNA polymerase II in atomic details: implications of hydrogen bonds between protein loops and DNA

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RNA polymerase II (RNAPII) is a macro-molecular complex that synthesizes RNA by reading the DNA code, a process called transcription. During the initiation step of the transcription, the RNAPII opens the double-stranded DNA in order to read the DNA code. Since the formation of the DNA transcription bubble remains poorly understood, we used molecular dynamics simulations to provide atomic-level insights into this crucial step of transcription.

Here, by steering the simulations with a combination of (i) guided DNA rotation and (ii) path collective variables [1], we obtained for the first time continuous atomic trajectories of the complete DNA opening process. The simulations provide insights into the role of loop dynamics and protein-DNA interactions during DNA opening.

[1] Branduardi, D.; Gervasio, F. L.; Parrinello, M. From A to B in free energy space. The Journal of Chemical Physics2007,126, 054103.