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Toward a Detailed Description of the Thermally Induced Dynamics of the Core Promoter BOIAN ALEXANDROV, Theoretical Division, Los Alamos National Laboratory, VLADIMIR GELEV, Beth Israel Deaconess Medical Center and Harvard Medical School, KIM RASMUSSEN, ALAN BISHOP, Theoretical Division, Los Alamos National Laboratory, ANNY USHEVA, Beth Israel Deaconess Medical Center and Harvard Medical School — Experimental data suggest that a spontaneous dsDNA strand separation at the transcriptional start site (TSS) is likely to be a requirement for transcription initiation in several promoters. We present molecular dynamic simulations of DNA to analyze the strand separation (bubble) dynamics of 80 bp long promoter DNA sequences. We suggest that three dynamic quantities: bubble probability, bubble lifetime, and average strand separation, together represent an adequate characterization of the bubble formation at TSS's of eight mammalian gene promoters. The TSS is distinguished by large, frequent, and *long-lived* transient openings in the double helix. In support of these results are our experimental transcription data demonstrating that an artificial DNA template, viz., a bubble-template of 5 bp mismatch at the TSS, is transcribed bi-directionally by human RNA polymerase alone in *the absence* of any other transcription factors.

Boian Alexandrov
Theoretical Division, Los Alamos National Laboratory

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