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Dynamic Coarse-Graining of DNA Melting Kinetics: Enthalpic and Entropic Effects of Cooperative Base-Pair Dynamics SEBASTIAN SENSALE, ZHANGLI PENG, HSUEH-CHIA CHANG, University of Notre Dame
— An MD dynamic coarse-graining approach is developed to analyze the correct melting kinetics of short DNA sequences. Existing models described well the thermodynamic melting temperature and near-equilibrium phenomena such as bubble formation and sharp phase transitions. However, the predicted kinetic rates were off by several orders of magnitude because they do not capture non-equilibrium coupled dynamics near the transition state like cooperative separation due to base stacking, hydration cage vibration and unwinding of the helix. By projecting onto the one-dimensional cooperative reaction coordinate, based on time-scale separation, we decipher the sequential triggering of several key events that determine the successive changes in enthalpy, vibrational entropy and configurational entropy towards the melting barrier. This results in a Fick-Jacobs type funnel transition state theory which allows us to use all-atomic simulations, Principal Component Analyses and elastic homogenization theory to identify the enthalpies and entropies at strategic locations along the reaction coordinate and to correctly estimate the melting rate.

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