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Validating a DNA Simulation Model through Hairpin Experiments MARGARET LINAK, KEVIN D. DORFMAN, University of Minnesota — We will present a comparison between large-scale melting experiments of DNA hairpins and the predictions of a coarse-grained BD computation model. Most computational efforts to date take a physical approach to modeling ssDNA. While this is effective for understanding the fundamental properties of self-interacting polymers, such studies are rarely related to laboratory experiments at biological conditions. To address this need, we have investigated DNA hairpins. The system emphasizes the role of stacking and hydrogen bonding energies, characteristics of DNA, rather than backbone bending, stiffness, and excluded volume interactions, which are generic characteristics of semi-flexible polymers. In conjunction with our melting curve experiments, we varied the temperature, hydrogen bonding, and stacking parameters in our model. The comparison of our simulation and experimental results provides a strong test of our model's suitability for capturing the sensitive behavior of simple hairpin systems. Furthermore, our approach and experimental data can be used to validate other similar coarse-grained simulation models.

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