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Molecular Rigidity and Entropy-Enthalpy Compensation in DNA Hybridization JACK DOUGLAS, FERNANDO VARGAS-LARA, Materials Science and Engineering Division, NIST, Gaithersburg, MD 20899 — Entropy-enthalpy compensation (EEC) is a general and relatively poorly understood pattern in the energetic parameters governing both binding constants and relaxation processes in condensed matter. After defining the basic phenomenology, we focus on how polymer additives, chain confinement, chain length variation affect a well-studied molecular binding process, the hybridization of duplex DNA. Our study is based on a coarse-grained model of DNA that does treat water explicitly. We find that both crowding due to polymer additives and geometrical confinement lead to a change of the effective chain rigidity and that changes in DNA generally lead to a pattern entropy-enthalpy compensation in the DNA association similar to experimental observations. Modulation of the rigidity of binding specifies by constraints associated with chain structure or environmental conditions can greatly influence both the location and cooperativity of molecular binding transition and the relative enthalpy and entropy contributions to the free energy of binding. Entropy-enthalpy compensation arises in numerous synthetic and biological molecular binding processes and we suggest that that changes in molecular rigidity might provide a common explanation of this ubiquitous phenomenon.

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