

## **Statistical Mechanics Models of Biomolecular Conformation.**

*Vassili Ivanov*

We are interested in developing reduced-degrees-of-freedom models of conformational transitions in biological macromolecules. For example, we have developed a statistical mechanics model for DNA melting in which base stacking and pairing are explicitly introduced as distinct degrees of freedom. Unlike previous approaches, this model describes thermal denaturation of DNA secondary structure in the whole experimentally accessible temperature range. Cooperativity arises from simple microscopic rules, as does the temperature dependence of the effective dimer free energies in the corresponding nearest neighbor thermodynamic model.

The partition function of the model can be written in a transparent transfer matrix form, and the model is exactly solvable in the homogeneous thermodynamic limit.

- V. Ivanov, Y. Zeng, and G. Zocchi, “Statistical mechanics of base stacking and pairing in DNA melting”, *Phys. Rev. E* **70**, 051907 (2004).
- V. Ivanov, D. Piontkovski, and G. Zocchi, “Local Cooperativity Mechanism in the DNA Melting Transition”, *Phys. Rev. E* **71**, 041909 (2005).