1099-92-357 **Sarah A Harris*** (s.a.harris@leeds.ac.uk), Leeds, LS2 9JT, United Kingdom, **Thana Sutthibuttpong**, Leeds, United Kingdom, **Agnes Noy**, Leeds, United Kingdom, and **Charles Laughton**, , United Kingdom. *Sequence Dependent Denaturation in Small DNA Circles: A Multi-scale Approach.*

The discovery of the structure of duplex DNA revealed how cells store genetic information. Small DNA circles offer a controllable model system for the systematic exploration of the dependence of DNA structure on supercoiling. We use computer simulation to explore the supercoiling-dependent conformation of small DNA circles and how this is affected by supercoiling. However, even given the most powerful supercomputers currently available, we are unable to perform fully atomistic simulations over sufficiently long timescales to gain adequate statistics to quantify patterns of sequence dependent denaturation due to supercoiling. Consequently, in ongoing calculations we are comparing the results of the atomistic models with statistical mechanical methods [1] and coarse-grained simulations [2].

[1] Mitchell J. S., Laughton C. A. & Harris S. A. Atomistic simulations reveal bubbles, kinks and wrinkles in supercoiled DNA. Nucleic Acids Res. 2011. 39: p. 3928-3938. [2] Sulc P., Romano F., Ouldridge T. E, Rovigatti L., Doye J. and Louis A. A. Sequence-dependent thermodynamics of a coarse-grained DNA model. J. Chem. Phys. 2012, 137, 135101. [3] Wang, H.Q. and Benham, C.J, Superhelical Destabilization in Regulatory Regions of Stress Response Genes. PLoS Comp. Biol., 2008, 4, e17. (Received February 11, 2014)