1172-92-212 **Pei Liu***, 234 Vincent Hall, 234 Vincent Hall, Minneapolis, MN 55401. *Ion-dependent DNA Configuration in Bacteriophage Capsids.*

Bacteriophages densely pack their long dsDNA genome inside a protein capsid. The conformation of the viral genome inside the capsid is consistent with a hexagonal liquid crystalline structure. Experiments have confirmed that the details of the hexagonal packing depend on the electrochemistry of the capsid and its environment. We propose a model that quantifies the relationship between DNA configurations inside bacteriophage capsids and the types and concentrations of ions present in a biological system. We introduce an expression for the free energy which combines the electrostatic energy with contributions from bending of individual segments of DNA and Lennard–Jones-type interactions between these segments. The equilibrium points of this energy solve a partial differential equation that defines the distributions of DNA and the ions inside the capsid. We develop a computational approach that allows us to simulate much larger systems than what is possible using the existing molecular-level methods. In particular, we are able to estimate bending and repulsion between the DNA segments as well as the electrochemistry of the solution, both inside and outside of the capsid. The numerical results show good agreement with existing experiments and with molecular dynamics simulations. (Received August 29, 2021)