MAS17-2017-000005

Abstract for an Invited Paper
for the MAS17 Meeting of
the American Physical Society

DNA is an Active Force-Generating Element in a Viral Molecular Motor

STEPHEN HARVEY, University of Pennsylvania

Double-stranded DNA (dsDNA) bacteriophages have a protein coat (the capsid) surrounding a dsDNA genome. During viral assembly, an ATP-driven motor forces the DNA into the preformed capsid. These motors are among the strongest of all biological motors. We proposed that the DNA is an active component in the translocation machinery. This "scrunchworm hypothesis" argues that the portal proteins drive dsDNA through a cycle of shortening and lengthening, and that the DNA shortening-lengthening cycle is coupled to a protein-DNA grip-and-release cycle to rectify the motion and drive the DNA forward. We have recently completed computer simulations on the DNA-portal complexes from phages phi29, T4 and P22. We also examined the patterns of electrostatic potential in all the structures. We conclude that (1) conformational changes in the portal proteins drive lengthening and shortening motions in dsDNA in the portal's channel; (2) these DNA conformational changes are driven by protein-DNA electrostatic interactions; and (3) DNA shortening and lengthening motions play an active role in translocation. The challenges ahead include (1) identification of the conformational changes in the ATPase during the biochemical cycle; and (2) determining how these drive conformational changes in the portal.