

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Electrostatic Persistence Length in Polymeric and Biological Systems**<sup>1</sup> JAN-MICHAEL CARRILLO, Oak Ridge National Laboratory, ANDREY DOBRYNIN, ZHEN CAO, University of Connecticut — Electrostatic interactions play an important role in controlling properties of polyelectrolytes and biological objects, such as DNA and filamentous viruses. The change in the ionic environment in such systems can influence their conformational properties. Using molecular dynamics simulations and theoretical calculations we have developed a model of swelling of semiflexible polyelectrolytes in salt solutions. Our approach is based on separation of length scales which allowed us to split a chain's electrostatic energy into two parts that describe local and remote along the polymer backbone interactions. The local part takes into account interactions between charged monomers that are separated by distances shorter than the persistence length. These electrostatic interactions renormalize chain persistence length. The second part includes electrostatic interactions between remote charged pairs located at distances larger than the persistence length. These interactions are responsible for chain swelling. In the framework of this approach we calculated effective chain persistence length and chain size as a function of the Debye screening length, chain degree of ionization, bare persistence length and chain degree of polymerization. Our crossover expression for the effective chain's persistence length is in a good quantitative agreement with the experimental data on DNA. We have been able to fit experimental data sets by using two adjustable parameters: DNA ionization degree ( $\alpha = 0.15 \pm 0.17$ ) and a bare persistence length ( $l_p = 40 \pm 44nm$ ).

<sup>1</sup>NSF-DMR-1004576

Jan-Michael Carrillo  
Oak Ridge National Laboratory

Date submitted: 15 Nov 2013

Electronic form version 1.4