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Effect of the Electrostatic Interactions on Stretching of Semiflexible and Biological Polyelectrolytes JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Polymer Program, Institute of Materials Science, University of Connecticut — Using combination of the molecular dynamics simulations and theoretical calculations we have shown that the bending rigidity of biological and semiflexible polyelectrolytes is force dependent. The effective chain bending rigidity decreases with increasing the value of the applied force. At small and intermediate force magnitudes a semiflexible polyelectrolyte behaves similar to a neutral chain with the effective bending rigidity equal to the sum of the bare chain and electrostatic bending rigidities which has a well known Odijk-Skolnick-Fixman (OSF) form with a quadratic dependence on the Debye radius. However, in the limit of the large forces when the magnitude of the applied force exceeds an electrostatic force responsible for the local chain stretching the effective chain's bending rigidity is determined by the bare chain's elastic properties. This dependence is a result of the scale dependent effect of the electrostatic interactions on the chain bending and elastic properties that can be approximated by two characteristic length scales. One describes the chain's elasticity at the distances along the polymer backbone shorter than the Debye radius while another controls the long-scale chain's orientational correlations. By stretching a semiflexible polyelectrolyte one probes different chain's deformation modes.

Jan-Michael Carrillo
Polymer Program, Institute of Materials Science, University of Connecticut

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