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Confinement free energy of flexible polyelectrolytes in spherical cavities RAJEEV KUMAR, M. MUTHUKUMAR, UMASS, Amherst — A single flexible polyelectrolyte chain in a spherical cavity is analyzed using self-consistent field theory (SCFT) in the presence of solvent molecules and salt ions. It is found that the confinement of the chain leads to creation of a charge density wave along with the development of a potential difference across the centre of cavity and the surface. We have computed different energetic and entropic contributions to the free energy of the system. In particular, the role of wall-segment repulsive interactions and concentration fluctuations (at one loop level) in free energy has been explored. Results for the finite size corrections to free energy and osmotic pressure will be presented. Predictions about the effects of salt concentration, chain length, radius of the cavity, electrostatic interaction strength, degree of ionization and solvent quality will also be presented.

Rajeev Kumar
UMASS, Amherst

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