Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Unifying Self-Consistent Field Theory for Weak Polyelectrolytes

KEVIN WITTE, YOU-YEON WON, Purdue University — A self-consistent field (SCF) theory for weak polyelectrolytes has been derived from a grand canonical partition function. The formalism accounts for the location and mixing of the charged and uncharged polymer species, treating the local (spatially dependent) charge fraction as a field variable with which to minimize the total free energy. This method of the derivation gives the resulting equations, especially those governing the local charge fraction, that are identical to the results obtained by Szleifer and coworkers (J. Polym. Sci. B Polym. Phys., 2006) who built upon the mean-field "annealed" free energy expression proposed by Raphael and Joanny (Europhys. Lett., 1990). However, we show that these results are further identical to the "two-state" model of Borukhov, Andelman and Orland (Eur. Phys. J. B, 1998), namely, the potential field due to the polymer charges with which the chains interact and the local charge fraction are shown to be exactly equal. This annealed model is derived by averaging the partition function with regard to the monomer charges. The charged and uncharged states are weighted by their probabilities which is, in our notation, the bulk charge fraction and one minus the bulk charge fraction, respectively. The utility of this theory is demonstrated by comparing its predictions against various experimental results from bulk potentiometric measurements and also from polyelectrolyte brush compression studies.

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Date submitted: 27 Nov 2007 Electronic form version 1.4