

Supplementary information for “Role of charge regulation and fluctuations in the conformational and mechanical properties of weak flexible polyelectrolytes”

Pablo M. Blanco^{(a),*}, Sergio Madurga^(a), Claudio F. Narambuena^(b), Francesc Mas^{(a),*} and Josep L. Garcés^(c)

October 25, 2019

(a) Physical Chemistry Unit, Materials Science and Physical Chemistry Department & Research Institute of Theoretical and Computational Chemistry (IQTCUB) of Barcelona University (UB), Barcelona (Catalonia, Spain)

(b) Facultad Regional San Rafael, Universidad Tecnológica Nacional & Instituto de Física Aplicada (INFAP), Universidad Nacional de San Luis-CONICET.

(c) Chemistry Department. Technical School of Agricultural Engineering & AGROTECNIO of Lleida University (UdL), Lleida (Catalonia, Spain)

(*) correspondence: pmlblanco@ub.edu; fmas@ub.edu

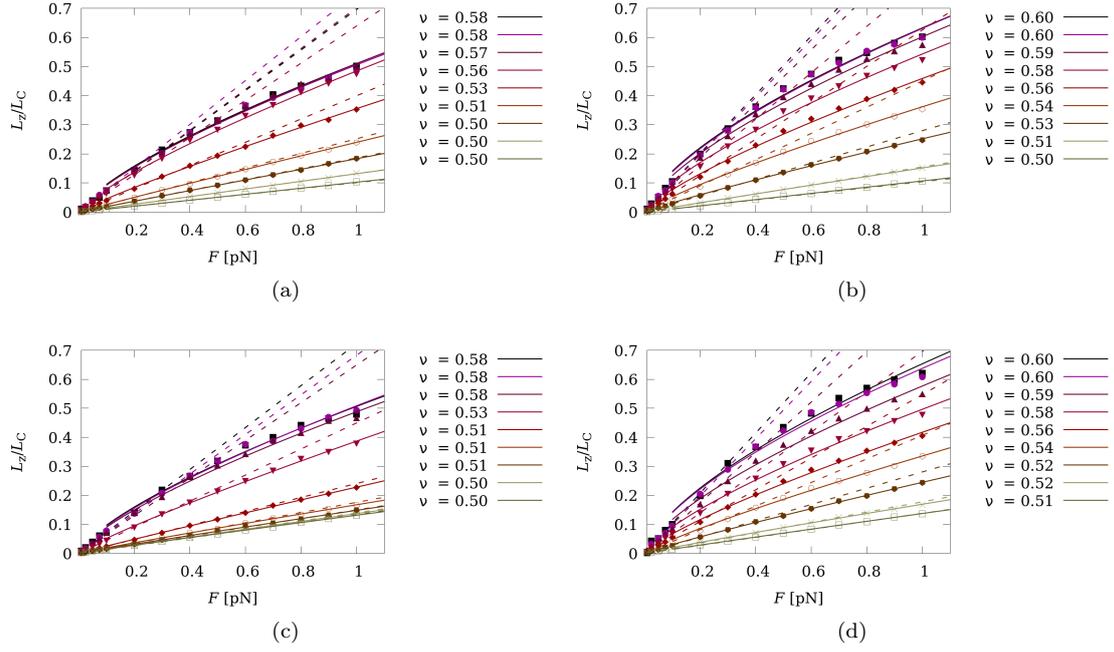


Figure 1: Force F vs. extension L_z curves in the low force regime obtained at different pH-values of 3 (light purple circles), 4 (dark purple upwards triangles), 5 (pink downwards triangles), 6 (red diamonds), 7 (ochre empty pentagons), 8 (brown filled pentagons), 9 (light green crosses) and 10 (empty squares). The markers show the ccMC (a and b) and the SMC (c and d) results with excluded volume (c and d) at two different ionic strengths of 1 M (left) and 0.001 M (right). The dashed lines follow the force/extension linear prediction whereas the continuous ones show the best fit of the computational data to the Pincus scaling law. L_z is normalized to the polyelectrolyte contour length $L_C = Nl_0 \cos((\pi - \alpha_0)/2)$.