

## Interfacial Adsorption of pH-Responsive Polymers and Nanoparticles

Shiyi Qin and Xin Yong

Department of Mechanical Engineering, Binghamton University, The State University of New York, Binghamton, New York 13902, United States

### Supplementary Table

**Table S1. DPD interaction Parameters between Different Components (in Units of  $k_B T/r_c$ )**

	water	oil	core	polyelectrolyte	counterion	salt
water	<b>25</b>	<b>100</b>	<b>75</b>	<b>25</b>	<b>25</b>	<b>25</b>
oil		<b>25</b>	<b>25</b>	<b>45</b>	<b>100</b>	<b>100</b>
core			<b>25</b>	<b>75</b>	<b>75</b>	<b>75</b>
polyelectrolyte				<b>25</b>	<b>25</b>	<b>25</b>
counterion					<b>25</b>	<b>25</b>
salt						<b>25</b>

### Supplementary Figures

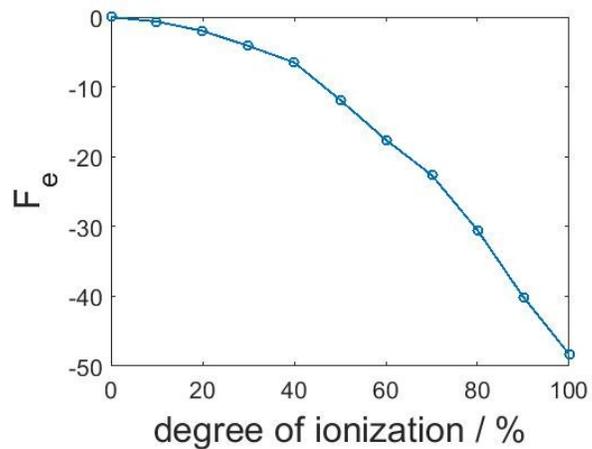


Figure S1. Instantaneous total electrostatic force applied on the linear polyelectrolyte in the direction perpendicular to the water-oil interface as a function of the degree of ionization of the polyelectrolyte. The polymer is placed parallel to the interface at a distance of 0.175 DPD length units.

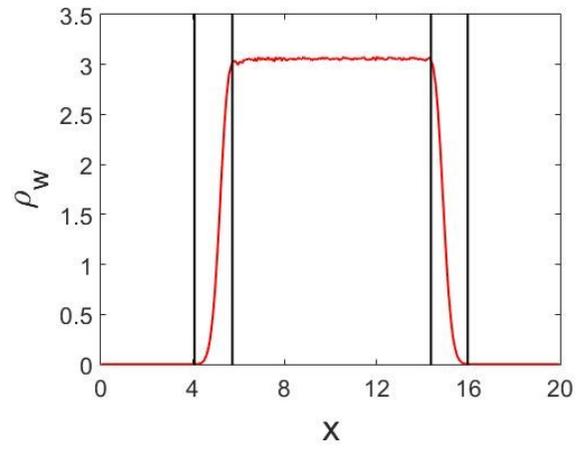


Figure S2. Density profile of water in the  $x$  direction. The four black solid lines define the positions and widths of interfacial regions for measuring the residence time.

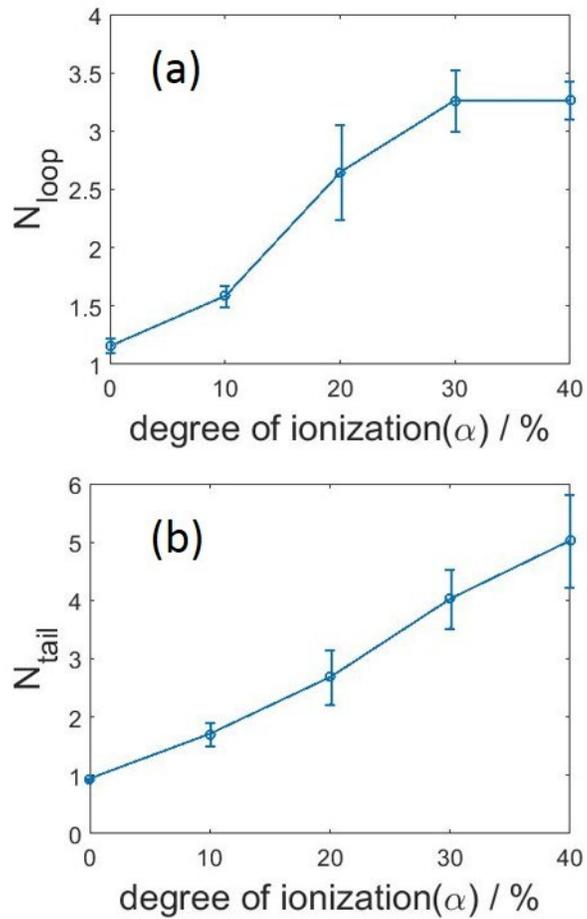


Figure S3. (a) Time-averaged number of beads in the loop segments as a function of degree of ionization (b) Time-averaged number of beads in the tail segments as a function of degree of ionization. The error bars in (a) and (b) represent the variations among four independent runs. The length of polyelectrolytes is  $L_c = 20$ .

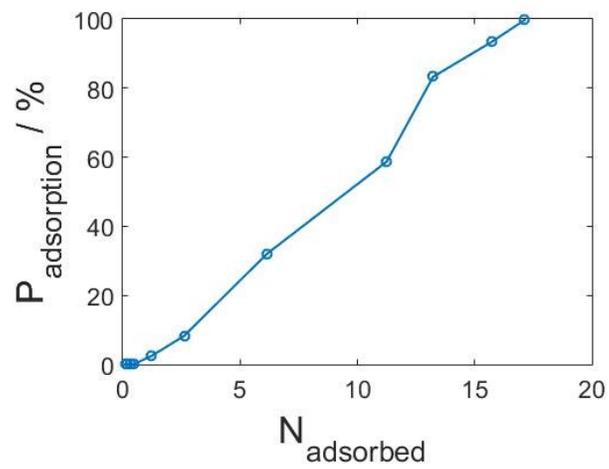


Figure S4. Probability of adsorption at the interface as a function of number of adsorbed beads for individual polyelectrolytes under different degrees of ionization. The length of polyelectrolytes in these simulations is  $L_c = 20$ .

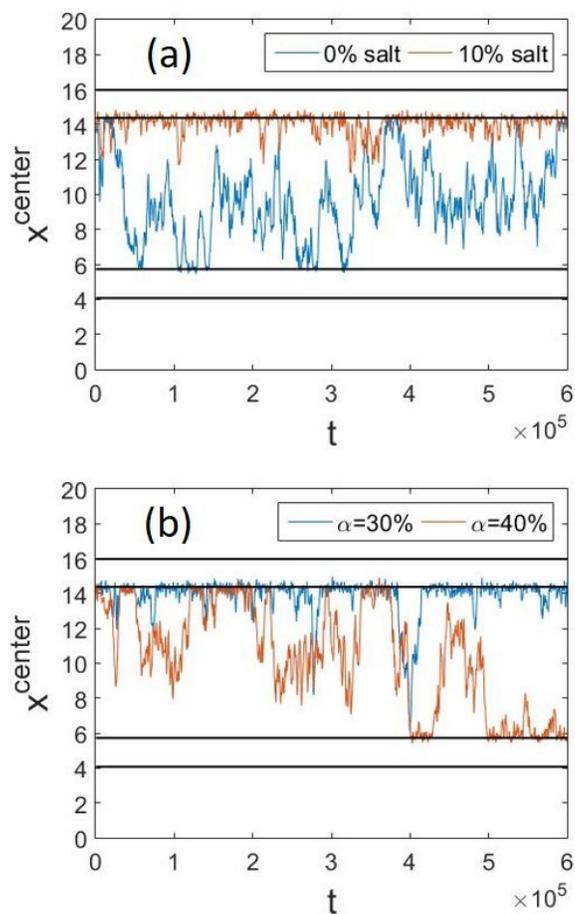


Figure S5. Time evolution of the  $x$  positions of the center of mass of the linear polyelectrolytes for the salt-free system and the system with 10% salt concentration. The degrees of ionization of polyelectrolytes are (a) 50 % and (b) 80 %.

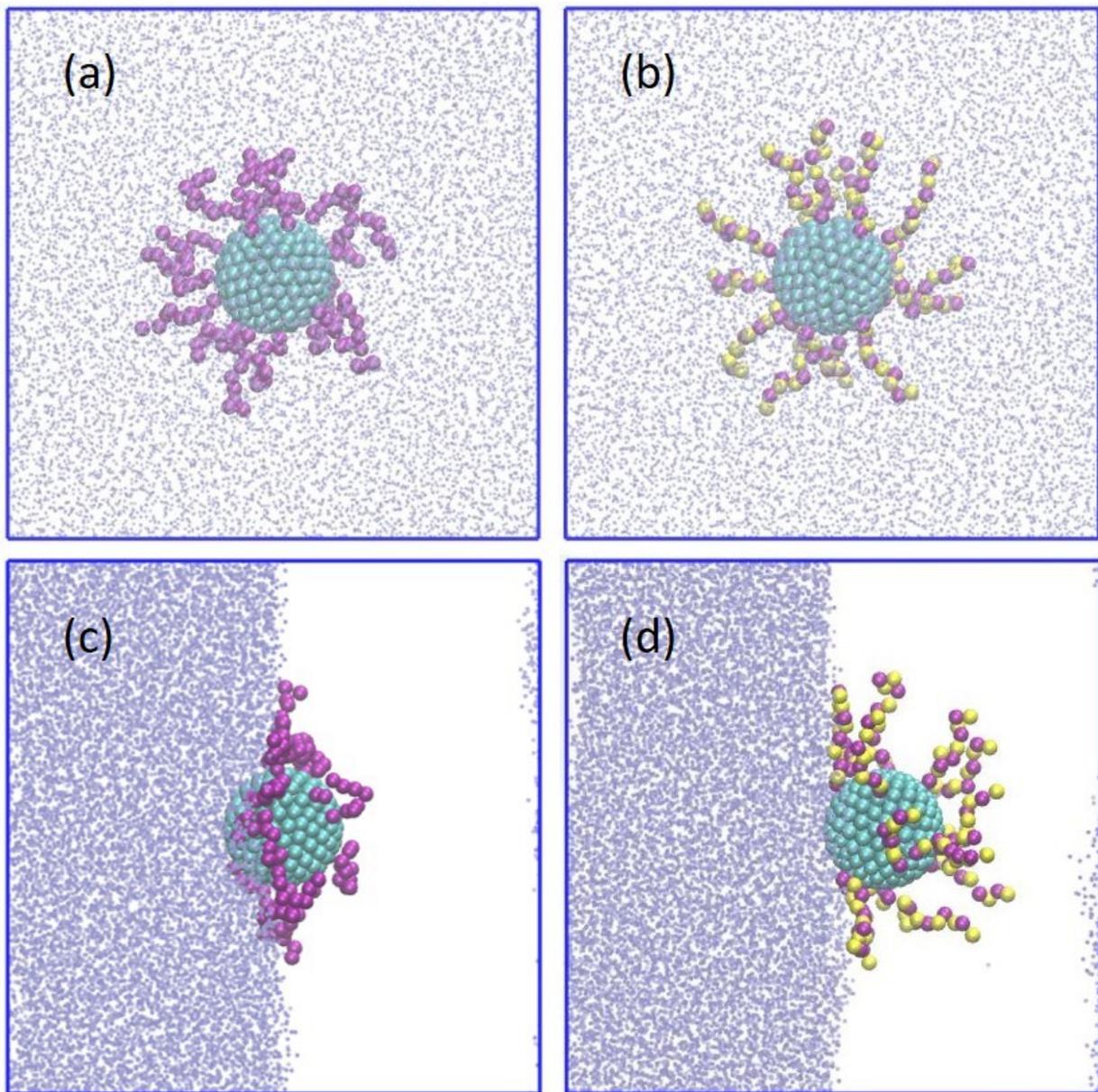


Figure S6. (a) Top view and (b) side view of the PNP with  $\alpha = 0\%$  adsorbed at the water-oil interface. (c) Top view and (d) side view of the PNP with  $\alpha = 50\%$  adsorbed at the water-oil interface. The length of polyelectrolytes grafted is 10.