Contribution ID: **26** Type: **Oral**

Adsorption of oligo-ampholytes to like-charged polyelectrolytes

Proteins are known to adsorb to polylelectrolytes on the "wrong" side of the isoelectric point, i.e. when the overall charge of the protein has the same sign as that of the polyelectrolyte. This has been attributed to patchy charge distribution on the proteins, whereas changes in their ionization upon adsorption have been neglected. In this work we show that the patchy charge distribution is not necessary if pH-responsive ionization of the charged groups is taken into account. We demonstrate it using a model system of a star-like anionic polyelectrolyte and an oligo-ampholyte, consisting of several acid (A) and base (B) groups. Using molecular dynamics simulations in the reaction ensemble show that the acid and base groups on a generic oligomer AAA-BBB adopt their ionization state to the local environment. Under suitable conditions, the negatively charged oligo-ampholyte in the bulk coexists with with its positively charged form adsorbed on the polyanion. Our simulations thus put forward a new paradigm for the interpretation of protein-polyelectrolyte interactions, and demonstrate that the changes in protein ionization must be taken into account. Furthermore, it provides a guideline for the design of bio-inspired oligo-ampholytes which would adsorb to polyelectrolytes under desired conditions, determined by the ionization constants, pKa and pKb of the ampholytes.

Preferred topic

Conformation of polymers in solvents

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