Metal cations in charge: Specific ion effects in soft matter systems

Ion specific effects are ubiquitous. The term denotes the fact that most processes in electrolyte solutions not only depend on ion concentration and valency, but also on the ion type.

In the first part of my talk, I provide insight into the origin of ion specific effects by combining results from molecular dynamics simulations and Poisson–Boltzmann theory at surfaces containing non-polar, polar and charged functional groups. This allows us to quantify ion-specific binding affinities to surface groups of varying polarity and charge, and to provide a connection to the experimentally measured long-ranged electrostatic forces that stabilize colloids, proteins and other biomolecules.

In the second part of my talk, I focus on the interaction of metal cations and RNA. To investigate the role of different cations in RNA folding and function, an accurate parametrization is crucial to capture the fine differences between distinct metal cations in classical all-atom simulations. Using enhanced sampling techniques allows us to capture rare events and slow processes like partial ion dehydration to form inner-sphere ion-pairs and to calculate ion binding affinities as well as kinetic rate coefficients.