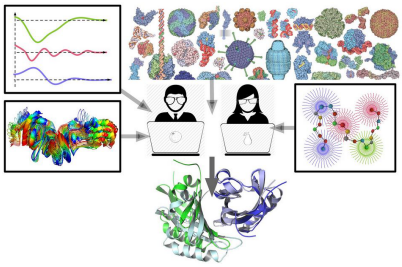

Contribution ID: **25** Type: **Oral**

Toward a refined electrostatic description for biomolecules simulations : introducing an effective pH and titration scheme to a coarse-grained nucleic acids model

Electrostatic interactions play a pivotal role in many (bio)molecular association processes. The molecular organization and function in biological systems are largely determined by these interactions from pure Coulombic contributions to more peculiar mesoscopic forces due to ion-ion correlation and proton fluctuations. By means of constant-pH Monte Carlo simulations based on a fast coarse-grained titration proton scheme,
a new computer molecular model was devised to study protein-RNA interactions and compute local pka values for RNA molecules.
Our results illustrate the importance of the charge regulation mechanism that enhances
the association between biological macromolecules in a similar way as observed for other protein-polyelectrolyte systems typically found in colloidal science. Due to the highly negative charge of RNA,
the effect is more pronounced in this system as predicted by the Kirkwood-Shumaker theory.
These efficient calculations have now been coupled to coarse-grained simulations of nucleic acids to include the role of conformational
changes. We will present our work to obtain pH-dependent coarse-grained nucleic acids simulations.

Primary author: Prof. PASQUALI, Samuela

Presenter: Prof. PASQUALI, Samuela

Session Classification: Session 2