Protein Electrostatics Berlin 2016

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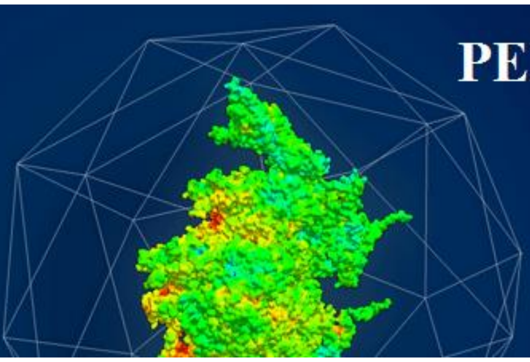

PEB 2016

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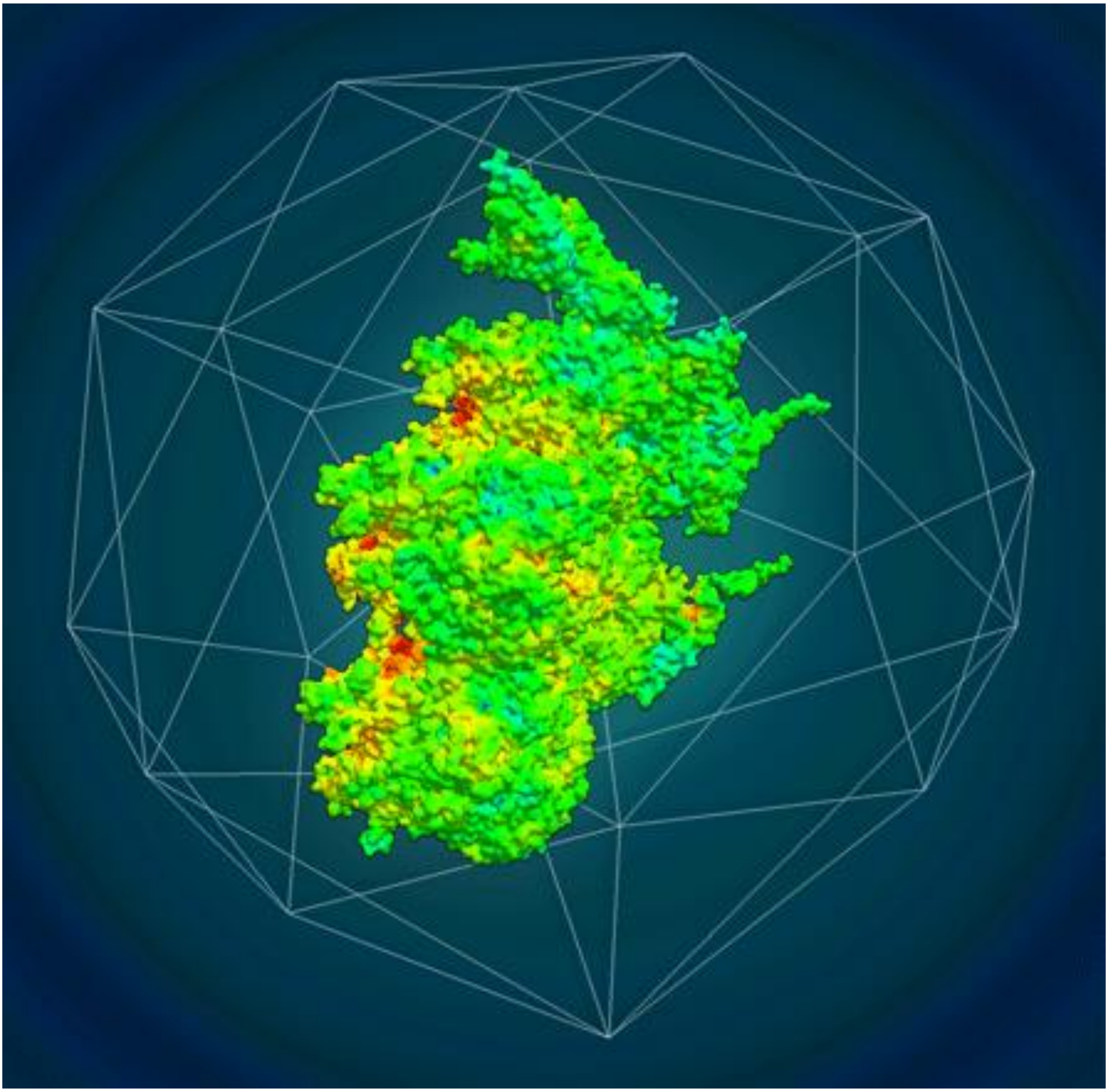

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Titratable Macroions in Multivalent Electrolyte Solutions

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In the world of proteins one can find exotic electrostatic phenomena such as long-ranged attraction between two electro-neutral protein particles in an aqueous solution, stemming from thermal charge fluctuations of dissociable charge groups on their surface. It was first observed by Kirkwood and Schumaker, half a century ago, who described it in the framework of statistical mechanical perturbation theory and showed that this interaction scales different from standard van der Waals interaction. Recently we have formulated a theory of fluctuation interaction between macroions subject to charge regulation and showed how the Kirkwood-Schumaker (KS) interaction follows directly from charge regulation, thereby generalizing the KS perturbation approach. Nevertheless, it has been a challenge to broaden a theory to be valid in the regimes where the original KS results fails, which is the case in strongly coupled electrolyte solutions. The experiments showed that the presence of multivalent ions can even enlarge this type of attraction between electro-neutral proteins.

Here we present a theoretical description of the effect of polyvalent ions on the interaction between titratable macro-ions. The model system consists of two point-like macro-ions with dissociable sites, immersed in an asymmetric ionic mixture of monovalent and polyvalent salts. We formulate a dressed ion strong coupling theory, based on the decomposition of the asymmetric ionic mixture into a weakly electrostatically coupled monovalent salt, and into polyvalent ions that are strongly electrostatically coupled to the titratable macro-ions. The charge of the macroions is not considered as fixed, but is allowed to respond to local bathing solution parameters (electrostatic potential, pH of the solution, salt concentration) through a simple charge regulation model. The approach presented, yielding an effective polyvalent-ion mediated interaction between charge-regulated macro-ions at various solution conditions, and describes the strong coupling equivalent of the Kirkwood-Schumaker interaction.