XIX Symposium on Condensed Matter Physics SFKM 2015

Book of Abstracts

7 – 11 September 2015
Belgrade, Serbia

Phenomenology Of Charge-Regulation Interaction In The Protein World

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Abstract. In the world of proteins one can find exotic electrostatic phenomena such as long-ranged attraction between two electro-neutral proteins in an aqueous solution, stemming from thermal charge fluctuations of dissociable charge groups on their surface, known as the Kirkwood-Schumaker (KS) interaction [1]. We present here an extension of KS theory, formulating it in a field-theoretical framework. Our model takes two small spherical macro-ions with dissociable charge groups, which are immersed in a monovalent salt solution. Fluctuating charge on a macro-ion's surface is regulated by local variables such as pH, salt concentration and local electrostatic potential. Charge regulation is described with the proper free energy function [2] for each of the macro-ions, while the coupling between the charges is evaluated at the approximate Debye-Hückel level. Strong attraction between like-charged particles is found close to the point of zero charge, specifically due to asymmetric and anticorrelated charge fluctuations of the macroion charges. The general theory is then implemented for a system of two protein-like macro-ions with known amino acid composition, generalizing the form and magnitude of the Kirkwood-Schumaker interaction. Results show that the strength of protein electrostatic interactions depends on the rate of change of the charge of the macro-ion with respect to the solution pH, i.e. the molecular capacitance of the macro-ion, which is protein specific [3, 4].

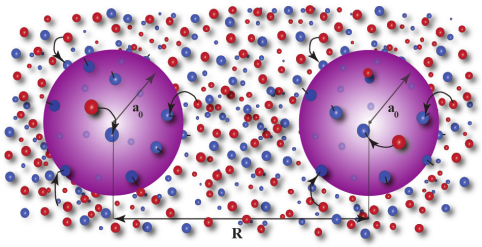

FIGURE 1. Two charge-regulated macro-ions, immersed in a solution composed of monovalent salt ions that can be exchanged with the surface sites.

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