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Presentation Abstract

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Abstract Title: ON THE DOMAIN OF APPLICABILITY OF CURRENTLY USED FORCE FIELDS FOR THE CALCULATION OF THE ACTIVITY OF ALKALI IONS AT PHYSIOLOGICAL IONIC STRENGTH

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Abstract Body: Alkali ions are present in virtually all biological processes. Their energetic properties have been so far predicted mostly by MD or MC calculations based on effective potentials derived for infinite diluted conditions (i.e. a single ion surrounding solely by water molecules) [1]. However, in physiological conditions, the concentration of K+ is sub-molar in the cytoplasm [2], and it may be by one, or even two, orders of magnitude larger near globular proteins or nucleic acids and in the active sites of of enzymes or channels [3-5]. The presence of a large ionic strength I is likely to limit the accuracy of the currently used potentials.

Here we will discuss recent calculations of the activity coefficients for K+,Na+ ions at increasing I. Such coefficients have been obtained by calculating the excess chemical potentials from thermodynamics integration [6], with several commonly used biomolecular force fields. Preliminary results show that classical force fields generally overestimate the activity coefficients of ions.

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