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Abstract for an Invited Paper
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Ion Atmosphere Near Nucleic Acids[1]

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We will discuss allatom structure based model that explicitly includes ionic effects, i.e., electrostatic interactions with explicit magnesium ions and implicit KCl that allow us to carry out explicit solvent molecular dynamics simulations of adenine riboswitch and SAMI riboswitch. Our predictions for the excess ions around the riboswitch, and the magnesiumRNA interaction free energy will be compared with experimental data. We will provide upper and lower bounds for preferential interaction coefficient, a statistical mechanical quantity that is a measure of excess ion atmosphere around a polyelectrolyte. We will discuss the role of surface charge density of mobile ions from added salt in determining the counterion release entropy associated with chain collapse. Finally, the Poisson's ratio of oligomeric DNA will be determined. (Work done in collaboration with R. Hayes, J. Noel, P. Whitford, S. Hennelly, J. Onuchic, and K. Sanbonmatsu.)

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