

PHYSIKALISCHES KOLLOQUIUM

des Fachbereichs Physik der Johann Wolfgang Goethe-Universität Frankfurt

> Mittwoch, den 27.06.2018, 16 Uhr c.t. Großer Hörsaal, Raum _0.111, Max-von-Laue-Str. 1



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"Metal cations and RNA a highly charged problem with a dynamic future"

Ribonucleic acid (RNA) is one of the most diverse biomolecules on Earth. RNA molecules are much more than information carriers between the DNA and the proteins. They play key roles in every vital process including protein synthesis and transport or gene expression. However, RNA molecules are highly charged polymers. Therefore, they can only fold into a compact and functional structure in the presence of positively charged ions.

Our research focuses on the role of metal cations in the folding and function of RNA. Resolving the role of metal cations is challenging experimentally since the resolution is typically insufficient to characterize the exact interactions. Here, computational methods such as molecular dynamics simulations can contribute significant insight. However, these simulations are challenged by the fact that they have to cover a broad spectrum of time scales ranging from femtoseconds to minutes and hours.

As a way to quantitatively describe cation-RNA interactions, I will discuss optimized atomistic models for the metal cations. These optimized models in combination with advanced sampling techniques allow us to resolve ion specific effects and to gain atomistic insight into the kinetics of cation binding. Subsequently, I will discuss the role of different metal cations in systems of increasing complexity starting from small structural RNA motifs and ranging to large and biologically relevant RNA macromolecules.

Die Dozenten der Physik

local host: Jun. Prof. Dr. Marc Wagne, mwagner@th.physik.uni-frankfurt.de