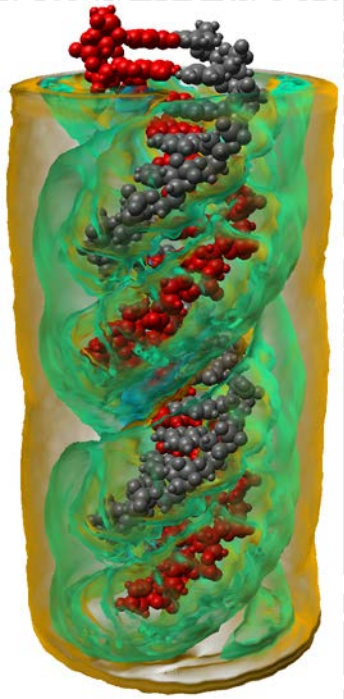
PHYSIKALISCHES KOLLOQUIUM

AM 15. JULI 2019 UM 17 UHR C.T.

IM GROßEN HÖRSAAL



HOW TO MODEL DNA TRANSLOCATION THROUGH NANOPORES – A MULTISCALE SIMULATIONAL EXPLORATION

PROF. DR. CHRISTIAN HOLM

INSTITUTE FOR COMPUTATIONAL PHYSICS,
UNIVERSITY OF STUTTGART

In this talk I will describe our efforts to understand the current modulations a double-stranded DNA will produce when it translocates in an electrolyte bath of varying concentration via an externally applied electric field through a nanopore device. The complete understanding of this electrokinetic process is important to develop novel DNA sequencing tools, or to use the nanopore as a sensor device for various macromolecular analytes. There are by now already commercial applications of such nanosequencers available.
Understanding can be gained on various length scales, and to this end we will start with atomistic simulations of dsDNA in explicit water. The comparison with experimental results helped us in constructing an accurate electrokinetic coarse-grained model for dsDNA. Going to even larger length scales requires the usage of continuum theories which can help us to understand the electrokinetic transport of charged macromolecules through millimetre long glas nanocapillaries.