CARL VON OSSIETZKY universität OLDENBURG
FAKULTÄT V
MATHEMATIK UND NATURWISSENSCHAFTEN

Institut für Physik

Theoriekolloquium

Am **14. November 2019** um **14.15 Uhr** in **W2 1-143** hält

Herr Prof. Dr. Ilia Solov'yov

einen Vortrag mit dem Titel

Theoretical and computational approaches for studying quantum effects in biological systems

Computational modeling of cellular processes at the molecular level has become crucial for laboratory and clinical studies to battle disease. No longer limited by small, single-protein systems or irrelevantly short timescales, molecular modeling currently permits exploration of a vast range of length and timescales from quantum biological processes to cell-scale organization and dynamics. The degree of realism reached lets us truly consider the computational approach to be a new kind of microscopy. In this presentation I will discuss some emerging tools of computational microscopy and present several case studies of biophysical processes that could benefit significantly from simulations.
I will first introduce VIKING (Scandinavian Online Kit for Nanoscale Modeling) - an online service uniting modeling tools through a powerful user-friendly interface and giving a unique opportunity to perform multiscale simulations. Next I will discuss software currently included, and planned for integration in VIKING. I will specifically focus on MesoBioNano Explorer, which is a multi-purpose package developed to model molecular systems of varied levels of complexity. I will summarize by demonstrating how the introduced programs could be used to describe several supra-molecular phenomena relying on electron dynamics.

Interessierte sind herzlich eingeladen.