

## Einladung zur öffentlichen Defensio von

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Thema der Dissertation:

## Modeling and Simulation of Field-Effect Biosensors

Abstract:

In this thesis we provide a general mathematical concept to deal with sensors with DNA-modified insulator-electrolyte interface. For that we describe the functioning of the system as a whole and suggest corresponding segmentation for further treatment as well as the compilation procedures for previously segmented model. Besides a mathematical analysis of partial differential equations occurring in the model the main focus of the work is the modeling and simulation of the processes that occur in the bio-physical part of the sensors.

The simulation of the bio-functionalized surfaces poses special requirements on the Metropolis-Monte-Carlo simulations and these are addressed by the algorithm. The constant-voltage ensemble enables us to include the correct boundary conditions.

We also identify the binding efficiency of the receptors to the DNAs of interest. For that we investigate the diffusive transport of the charged biomolecules and the two types of the chemical reactions near the functionalized surface, i.e. specific and non-specific binding.

Furthermore, an approach is developed for device characterization that allows to determine the biological noise of the system and to identify the signal-to-noise ratio. We focus on the stochastic processes that occur at the functionalized surface. The chemical Langevin equation for a binding (i.e. association and dissociation) processes occurring at the functionalized surface is obtained. The binding efficiency of the biomolecules, the signal and the biological noise of the device are specified and calculated.

Prüfungssenat:

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Zeit: Freitag, 08. Juli 2011, 11:00 Uhr

Ort: Fakultät für Mathematik, Seminarraum C 209, Nordbergstrasse 15