



Design principles for whole cell biosensors

Experimental study of Cell-cell interactions in thin inorganic matrices



The tight fixation of living cells inside of inorganic matrices while preserving their viability is a prerequisite for the development of bio-hybrid sensor-actor materials. Thereby, the knowledge of the particular conditions by which the different cell types retain their functionality for a long time remains of basic interest. The estimation of relevant parameters like cell vitality, cell to cell distances, porosity of the matrix or diffusion of signal molecules will be the aim of this study.

The **research plan** will include:

- 1. Fabrication of thin sol-gel layers with embedded yeast or bacterial cells (or spores) and estimation of the cell viability in dependence of storage conditions and time.
- Basic understanding of the relationship between cell to cell distances, porosity of the matrix, nutrition and survival of the cells.
- 3. Estimation of the optimum geometry and functionality for a simple sensor model system.

For further information please contact:





Pyroelectric disinfection of bacteria cells

Experimental study of disinfection of pyroelectric composite materials



Materials which are pyroelectric show the ability to generate a temporary electric potential by heating or cooling them. The electric potential inhibits the growth of microorganisms such as bacteria, fungi, algae or it can even kill them. Immobilized into filters or onto carriers, these crystals are applicable as disinfection tool e.g. in drinking water tanks, swimmingpools, or on labbenches.

The research plan will include:

- Immobilization of pyroelectric crystal powder (LiNbO₃, LiTaO₃) on organic matrices (e. g. alginate, collagen) in order to create porous pyroelectric filter material
- 2. Investigation of the pyroelectric properties of this composite material depending on particle size of pyroelectric powder
- Testing the pyroelectric filter due to the effect of disinfection

For further information please contact:



Manipulation of organic molecules by LT-STM

Experimental study of organic molecules by Scanning Tunneling Microscope (STM) at low temperature





Experimental STM images of PTCDA (R. Temirov *et al.,* New J. Phys. **10,** 053012 (2008))

Low Temperature STM (LT-STM) allows the manipulation of atoms and molecules. Experiments permit a deeper insight into the quantum electronics of molecular systems and provide important information on the conformational and mechanical properties of single complex molecules. The present project will be centred on the manipulation of individual molecules to quantitatively characterize the charge transport through a molecular unit. The **research plan** will include:

- Basic understanding of the electronic and structural properties of the relevant metallic surfaces and organic molecules
- 2. Basic understanding of Ultra-High-Vacuum (UHV) and Scanning Tunneling Microscopy
- 3. Probe preparation in UHV and molecular deposition
- 4. Imaging and manipulation of single molecules on metallic surfaces.

For further information please contact:





Metallo-organic nanostructures

Theoretical study of Scanning Tunneling Microscope (STM) experiments on organic molecules: a density functional theory approach

Goal of this thesis will be the investigation of the binding, and simulation of STM images, of organic molecules (PTCDA, fullerenes, phthalocyanines, organic photodiodes, etc.) on metallic surfaces.



PTCDA on Ag (111), with image of LDOS of LUMO (as would be observed in STM)

The research plan will include:

- 1. Basic understanding of the electronic and structural properties of the relevant metallic surfaces and organic molecules
- 2. Perform geometry optimizations of the the molecules chemisorbed (bonded) to metallic surfaces
- 3. Calculate DOS and simulate STM images using DFT combined with Tersoff-Hamann approximation
- 4. Investigate possible switching mechanisms for nanoelectronic devices formed from these structures

For further information please contact:





Transport properties of molecular switches

One of the main challenges of the research within the realm of nanoscience and nanotechnology is the ability to control conformations at



the molecular scale. One typical example are molecular switches, where the conformation of the molecule can be modified by light irradiation or mechanical actions. Goals of the thesis are the study of the transport properties of such switches.

The research plan will include:

- 1. Becoming familiar with the applications of molecular switches in nanoelectronics
- 2. Learning the basics of density functional tight binding calculations for the electronic structure
- 3. Learning the basics of quantum transport
- 3. Computing charge transport through molecular switches in different conformations

For further information please contact:





Controlling the electrical properties of nanoscale field-effect transistors

The size in electronic components such as transistors and capacitors is reducing down to the scale (around 10nm) where quantum effects become significant. At this



lengthscale conventional models of continuous media don't work anymore. Thus for the further development of electronic devices, the understanding of charge transport at the atomic scale including quantum effects is required. For this purpose, electronic devices such as field effect transistors (FETs) are modeled and the charge transport through the devices is investigated using atomistic descriptions. The **research plan** will include:

- 1. Modeling and relaxation of FET devices.
- 2. Calculation of electronic properties of FET devices in tight-binding model.
- 3. Simulation of I-V characteristics with different gate voltages using quantum transport theory within the Green function formalism.
- 4. Investigation of the homogeneous and inhomogeneous gate field effect on the transport properties.
- Investigation of the influence of impurities, surface roughness, the shape of the devices, and surface modifications on I-V characteristics.

For further information please contact:



Understanding mutations

The conformational dynamics in bio-molecular systems (DNA, proteins, etc) can play an important role in promoting or hindering electron or hole propagation through such systems. This is a crucial issue since *e.g.* DNA damage repair occurs via electron transfer processes. It is thus of interest to investigate the propagation properties of a charge injected into a fluctuating bio-molecule. In this thesis we will study model systems able to mimic such dynamical processes.





The research plan will include:

- 1. Becoming familiar electron transfer in DNA oligomers
- 2. Learning how to solve the time-dependent Schrödinger equation with static potentials.
- 3. Extend this to the case of time dependent fluctuating potentials to mimic the DNA conformational dynamics
- 4. Study the case of a linear chain where the fluctuations of the electronic parameters are drawn from molecular dynamics simulations.

For further information please contact:





Boron Nanostructures

Theoretical study of physical properties of boron nanostructures



Nanomaterials are in the focus of research worldwide. A new and very promising class of materials are boron nanostructures in form of sheets, nanotubes, fullerenes, nanowires, nanoribons, etc. Many of their properties still need to be determined. The goal of this thesis is to study the physical properties of boron nanotubes by means of theory. Your results will provide important information used to identify boron nanostructures in the lab.

The research plan will include:

- 1. Learning the basics of carbon and boron nanostructures
- 2. Learning the basics of density functional theory (DFT).
- 3. Get introduced to the operation of a DFT code (SIESTA, VASP, DFTB).
- 4. Performing DFT calculations of boron nanostructures to determine their basic electronic properties.
- 5. Study vibrational, optical or transport properties

For further information please contact:





Organic electronic materials

Theoretical study of the structureproperty relation of molecular organic semiconductors

Converting sun light into electricity with thin film organic semiconductors is receiving increased interest by the industrial sector at the moment.

In organic electronic devices, various conjugated molecules such as polycyclic aromatic hydrocarbons: tetracene, pentacene; oligothiophenes and their derivatives are used to build the transport layers and organic dyes for the absorber layers. The most important characteristic of the molecular semiconductors is the charge carrier mobility.

Theory is expected to play a major role in the understanding of the structure-property relationship with respect to the mobility. The goal of this thesis is the theoretical investigation of charge transport parameters of different experimentally studied organic molecular semiconductors.

The research plan will include:

- 1. Learning the fundamentals of molecular dynamics simulations and ab initio calculations.
- 2. Modeling thin films of different classes of organic functional materials.
- 3. Calculation of charge transport parameters and the charge carrier mobility with different techniques.

For further information please contact:



complex naterials

master thesis

Efficient energy conversion at the molecular level

theoretical study of thermoelectric figure of merit of molecular junctions

Inspired by the recent developments in molecular electronics, which is involved in understanding charge transport



properties of molecular systems, thermoelectric properties of molecular systems is now becoming a focus of nanoscience. Pioneering experiments show that molecular junctions can give large values of thermoelectric figure of merit, so they can be used as efficient energy conversion devices. The goal of this thesis will be theoretical investigation of thermal as well as charge transport at the quantum level, and exploring the material dependent properties that influence the conversion efficiency.

The **research plan** will include:

- 1. Basics of modeling electronic and vibrational properties of nano-scale systems.
- 2. Getting introduced to quantum transport theory and becoming familiar with Green function techniques.
- 3. Inclusion of impurity and surface roughness effects and the influence of geometrical modulations.
- 4. Investigation of methods to increase the thermoelectric figure of merit at molecular junctions.

For further information please contact:



Modeling fuel cells

theoretical study of the adsorption of water on platinum oxides



complex

Interaction of water with platinum oxides is of great interest in many respects as e.g. in fuel cells, in vehicle exhaust catalysts, and for assessment of consequences due to environmental pollution by platinum. Nanosized platinum clusters are covered by a thin oxide layer. Interaction of those clusters in wet environment could lead to dissolution of platinum and formation of undesired platinum complexes. For a basic atomistic understanding of this process, the interaction of water molecules with platinum oxides has to be clarified. In a first step, adsorption mechanisms of water on platinum oxides shall be elucidated by density-functional calculations.

The research plan will include:

- 1. Becoming familiar with ab initio calculations of atomic structures by means of density-functional theory.
- Total energy calculations with structure relaxation for different positions of water adsorbed on oxidized platinum surfaces.
- 3. Investigation of the adsorption pathways and the associated energy profiles of water molecules on reactive surface sites determined in 2).
- 4. Investigation of the effect of the water coverage (from single molecules to liquid water) on the adsorption mechanisms in 3).

For further information please contact: