master thesis

STM studies of molecules for molecular electronics

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

Low Temperature STM (LT-STM) allows deep insights into the electronic properties of molecular systems and provide important information on the conformational and mechanical properties of single complex molecules. The present project will be centered on the manipulation of individual molecules to quantitatively characterize the charge transport through a molecular unit.

The research plan will include:

1. 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.

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A novel research line at the Max Bergmann Center of Biomaterials includes the development and application of biomimetic hydrogels as microscopic experimental platform to perform and study biological function in a cell-like environment. In this thesis the aim is to identify new saccharide-based building materials to provide a biocompatible, non-toxic environment in which cellular function can be rationally studied. The applicant should have basic synthesis skills, be familiar with fluorescence microscopy and polymer chemistry / physics as well as microfluidics (design / fabrication / application).

The research plan will include:
1. Set-up synthesis to design novel saccharide-based pre-polymers
2. Fabricate microscopic hydrogels employing droplet-based microfluidics
3. Characterize polymer hydrogels (e.g. pore size via fluorescent probe diffusion)
4. Functionalize hydrogels with biomolecules (DNA)

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master thesis

Biological function in biomimetic hydrogels

Cell extracts as base material for in vitro transcription / translation outperforming commercial bio-kits

A novel research line at the Max Bergmann Center of Biomaterials includes the development and application of biomimetic hydrogels as microscopic experimental platform to perform and study biological function in a cell-like environment. In this thesis the aim is to design and fabricate a “home-made” in vitro transcription / translation kit from E. coli bacteria that will be later introduced in polymer hydrogels to mimic cellular complexity. Knowledge in cell-lysate extraction and molecular biology are key requirements.

The research plan will include:
1. Extract cell lysate from E. coli cells
2. Optimize buffers and reagents to design an in vitro transcription / translation kit
3. Test performance via production of deGFP in plate reader experiments and compare with commercial protein production kits (e.g. 5 Prime / Roche)

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master thesis

Biological function in biomimetic hydrogels

Long-term storable bio-kits

A novel research line at the Max Bergmann Center of Biomaterials includes the development of saccharide-based hydrogels as matrix material for prolonged storage of commercial bio-kits (e.g. for gene expression). In this thesis the aim is to design and synthesize micro- and macroscopic hydrogels and study their material properties (swelling, pore size) upon freeze drying. Thereafter, commercial bio-kits will be introduced in the polymer hydrogels and their shelf-life studied. Knowledge in molecular biology and basic polymer chemistry / polymer physics are key requirements.

The research plan will include:

1. Identification of promising saccharide-based pre-polymers
2. Synthesis and purification of pre-polymers, hydrogel formation
3. Freeze-drying of hydrogels – material characterization (e.g. SEM)
4. Introduction of bio-kits in hydrogels; study of storage properties with/without stabilizing matrix material

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master thesis

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
4. Computing charge transport through molecular switches in different conformations

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master thesis

Modeling of Polymer Wrapping Around Carbon Nanotubes

Carbon nanotubes (CNTs) are obtained as a mixture of nanotubes with different diameters and chirality (rolling direction). These nanotubes have different electronic and optical properties which is a unique feature of carbon nanotubes. For some application a separation of CNTs having particular diameter and chirality is necessary. One of the most promising method for such a separation is realized by wrapping of a particular polymer around a CNT of particular diameter. Though this method is already used for the separation of CNTs, the underlying mechanism is not fully understood yet. The aim of this study will be to perform a computer modeling of the wrapping of polymers around CNTs and to shed the light on the underlying effects to be able to control the CNT separation for their future applications. This work will be done in close collaboration with experiments and is a part of a scientific project supported by the EU.

The research plan will include:

1. Learning the basics of carbon nanotubes.
2. Learning the basics of density functional theory (DFT) and molecular dynamics (MD).
3. Get introduced to the operation of MD codes.
4. Creating atomic structures of different CNTs and polymers.
5. Performing large-scale MD calculations CNTs with polymers to model wrapping.
6. In addition the change of electronic and optical properties of CNTs induced by interaction with polymers can be investigated.

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master thesis

Synthesis of Doped Carbon Nanotubes for Applications in Biosensors and Gas Sensors

Nanomaterials and in particular carbon nanotubes (CNTs) are in the focus of research worldwide. A new and very promising method to modify and control physical and chemical properties of CNTs is doping of CNTs with N or B atoms during their synthesis. Such nanotubes are expected to be perfect active elements of novel sensors developed at our chair. The goal of this work is to fabricate N- and B-doped carbon nanotubes by means of CVD reaction and characterize them by means of the state of the art methods. The work will be done in close collaboration with two other groups working on integration of novel nanoscaled materials into the biosensors and gas sensors.

The research plan will include:

1. Learning the basics of carbon nano-structures
2. Learning basics of the CVD synthesis
3. Synthesis of N- and B-doped CNTs
4. Learning basics of physical characterization of nanomaterials
5. Sample preparations for characterisations
6. Characterisation tools: IR and Raman spectroscopy, SEM, TEM, EDX, EELS and AFM

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master thesis

Modeling and characterization of field-effect transistors for chemical sensor applications

Chemical/bio sensors consisting of nanostructures such as carbon nanotubes and silicon nanowires have been getting scientific and industrial attentions because of their high sensitivities, low cost and quick diagnosis. For further development of such sensing devices the understanding of the charge transport through the sensors including quantum effects is required. For this purpose, electronic devices such as field effect transistors (FETs) will be modeled theoretically and the electric properties are characterized. In addition, the influential factors controlling electron transport through the devices is investigated in close collaboration with in-house experiments. The research plan will include:

1. Modeling of FET devices with TCAD softwares (COMSOL).
2. Calculation of electric properties such as I-V characteristics and on-off ratios of FET devices using quantum transport theory. Investigation of AC and/or DC working modes.
3. Investigation of the influence of pH, ionic concentrations, and surface functionalization to the performance of the sensors.

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master/diploma thesis

Electronic and Transport Properties of two-dimensional Carbon- and Silicon-based Materials

Carbon nanotubes, graphene and silicene are only few examples of novel materials which are studied in our group regarding their electronic and transport properties. By using highly efficient numerical simulation methods, we investigate charge-transport characteristics of realistic samples of such materials under magnetic fields and/or under presence of typical defects [1-2] that are determined experimentally [3].

We offer possibilities for Master Theses related to the above topic and associated with our collaborative European network.

The research plan includes:
1. Getting familiar with transport codes and parallel numerical simulations.
2. Perform simulations of electronic transport in 2D graphene and silicene


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master/diploma thesis

Organic electronic materials

Theoretical study of the structure-property relation of molecular organic semiconductors

Converting sun light into electricity with thin film organic semiconductors is a highly important challenge in today’s research and society.

In organic electronic devices, various conjugated molecules such as polycyclic aromatic hydrocarbons: e.g. pentacene, thiophenes etc. and their derivatives are used to build the transport layers and host organic dyes for the absorber layers. One of 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 to finally improve solar cell efficiency.

The research plan will include:
1. Learning the fundamentals of molecular dynamics simulations and ab initio calculations.
3. Calculation of charge transport parameters and the charge carrier mobility.

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master/diploma thesis

Charge Transport through Topological Insulators

Topological Insulators [1] are a new class of materials which show fascinating properties and charge-transport characteristics. They have exceptional spin-polarized surface states which are robust to disorder (topologically protected) and which are currently in the focus of research groups worldwide, e.g. for their peculiar transport characteristics and localization phenomena.[2]

The envisioned Master Thesis project will focus on the study of transport phenomena in models of Topological Insulators.

The research plan includes:
1. Learning the fundamentals of Topological Insulators.
2. Getting familiar with transport codes and concepts of parallel numerical simulation.

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.

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master thesis

Pyroelectrocatalytic disinfection of bacteria cells

Experimental study of disinfection with Pyroelectric materials

LiNbO3 and LiTaO3 materials of polar crystal structure exhibit a spontaneous polarization that can be changed by temperature. This phenomenon, commonly known as pyroelectric effect, leads to the generation of surface charges that in turn are the source for a pyroelectrocatalytic or pyroelectrochemical activity of these materials. 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 should be applicable as disinfection tool e. g. in drinking water tanks, swimming pools, or on lab benches.

The research plan will include:

1. Development of pyroelectric layers and coatings with additional metallic nanoparticles
2. Characterisation of this layers, e. g. due to their morphology
3. Investigation of the pyroelectric performance and the disinfection properties

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master thesis

Characterization of target surfaces for photocatalysis

Experimental study of micro- and nanoscopic properties

The topic of this research is set into the context of the photocatalytical degradation of organic molecules. The photocatalyst has to be immobilized onto a target (surface). The interactions of target and photocatalyst (e. g. TiO2) will determine some of the properties of the photocatalytical process. Targets could be: glass, ceramic materials, polymeric substances and even fibres or garment.

The research plan will include:
1. Characterization of surfaces by imaging techniques (SEM, AFM …)
2. Exploration of surfaces by techniques of Materials Science (tribology …)
3. The aim is to give rules for a set of optimal materials dedicated for being covered by a photocatalyst

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master thesis

Characterization of immobilized photocatalysts

Experimental study of degradation properties

The topic of this research is set into the context of the photocatalytical degradation of organic molecules. Different immobilized photocatalysts have to be characterized according to their surface properties and their specific ability of degradation power. The methods in use are part of Materials Science and Physical Chemistry.

The research plan will include:

1. Implementation of a standard procedure for testing the photocatalytic power of immobilized photocatalysts
2. Investigations of the surface characteristics by means of tribology (e.g. scratch test)
3. Application of the standard procedure on given different immobilized photocatalyst specimen

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master thesis

Bacterial nanowires for biosensing devices

Experimental Studies

Bacteria have the potential to produce self-assembling appendices (such as pili or flagella) that can be used as biological nanowires. Here, we want to take advantage of these template structures and use them to build biosensors from pili and flagella.

The research plan will include:

1. Growth of different bacterial strains and optimisation of growth conditions,
2. Purification and metallization to gain conductivity,
3. Analysis of conductive and structural properties of bio-nanowires by atomic force microscopy, scanning electron microscopy and with predesigned microelectrodes

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