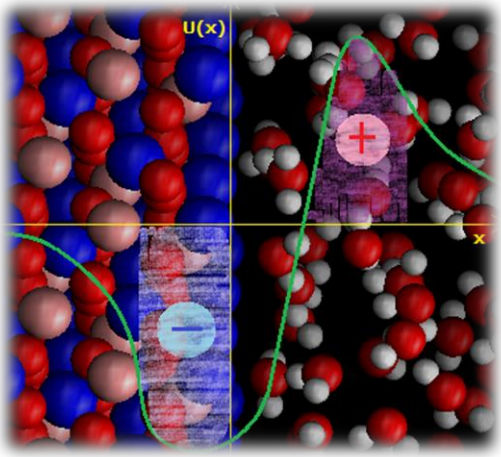
TECHNISCHE UNIVERSITÄT DRESDEN

complex nano materials

Master-/Diplomarbeit

Pyroelektrische Materialien in wässriger Umgebung

Theoretische Untersuchungen der Grenzflächeneffekte mithilfe Finite-Elemente-Methoden



An der Grenzfläche zwischen einem pyroelektrischen Festkörper und einer Elektrolytlösung laufen hochkomplexe elektrochemische Prozesse ab. Mit theoretischen Modellen der elektrischen Doppelschicht soll die räumliche Verteilung der Wassermoleküle in Abhängigkeit von verschiedenen Einflussparametern (z.B. Temperatur, Ionenkonzentration der Lösung) und materialspezifischen Eigenschaften (z.B. pyroelektrischer Koeffizient, Ladungsträgerdichte) untersucht werden. Eine Modellierung der ortsabhängigen Dichteverteilung und eine grafische Darstellung des Potenzialverlaufs im Bereich der Grenzfläche runden die Untersuchung ab.

Inhalt der Arbeit:

1. Weiterentwicklung der theoretischen Modelle aus der Literatur
2. Berechnung der physikalischen Größen mithilfe von Finite-Elemente-Methoden (praktische Erfahrungen mit FEM wären von Vorteil) unter Nutzung der entwickelten Modelle

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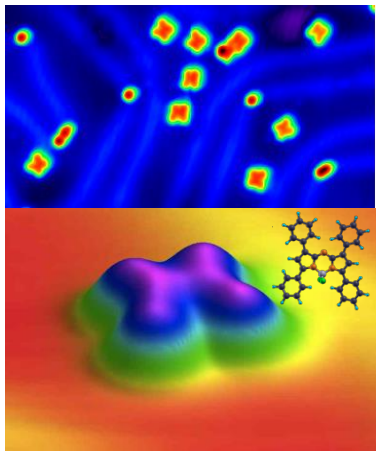
master thesis

STM studies of molecules for molecular electronics

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



Experimental STM images of Aza-BODIPY molecules

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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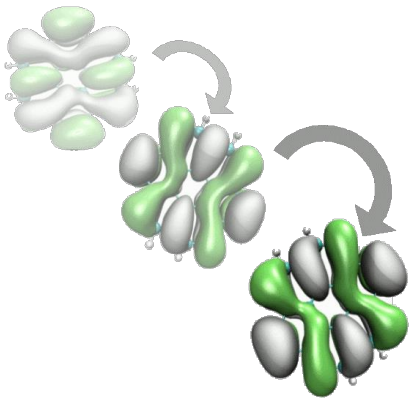

Organic electronic materials

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

Converting sun light into electricity
with thin film organic semiconductors
is a highly important challenge in todays 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 plays 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.
2. Modeling thin films and structures of different classes of organic functional materials.
3. Calculation of charge transport parameters and the charge carrier mobility.

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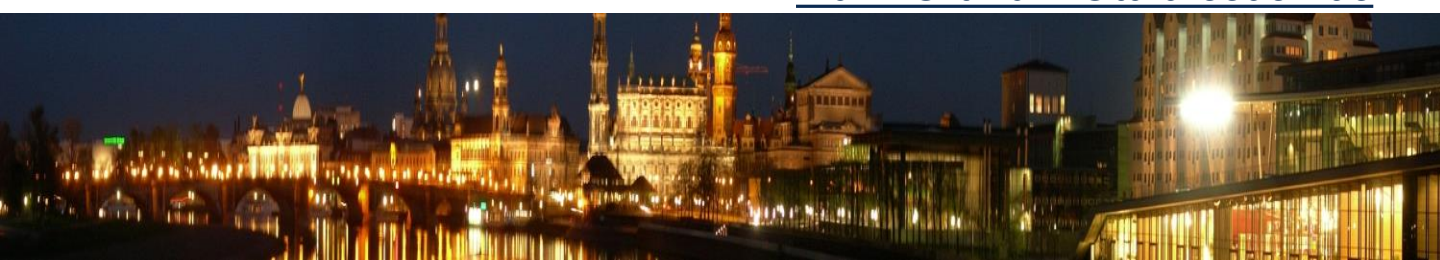

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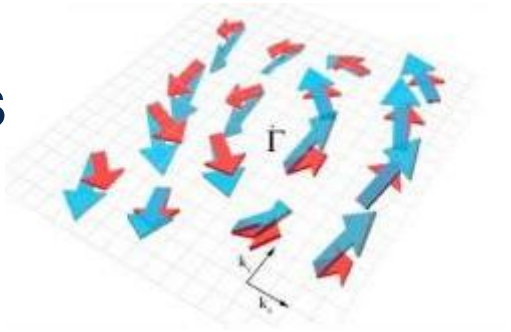

Charge Transport and Spin Effects in Topological Insulators

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 Diplom/Master Thesis project will focus on the study of transport phenomena and spin polarization in models of Topological Insulators.

The **research plan** includes:

1. Getting familiar with transport codes and concepts of parallel numerical simulation.
2. Perform simulations of spin effects on electronic transport in Topological Insulator films and/or wires.

Further Reading:

[1] M. Z. Hasan and C. L. Kane. Review of Modern Physics **82**, 3045 (2010).
[2] D. Soriano, F. Ortmann and S. Roche. Physical Review Letters **109**, 266805 (2012).
[3] D.V. Tuan, F. Ortmann et al. Nature Physics **10**, 857 (2014).

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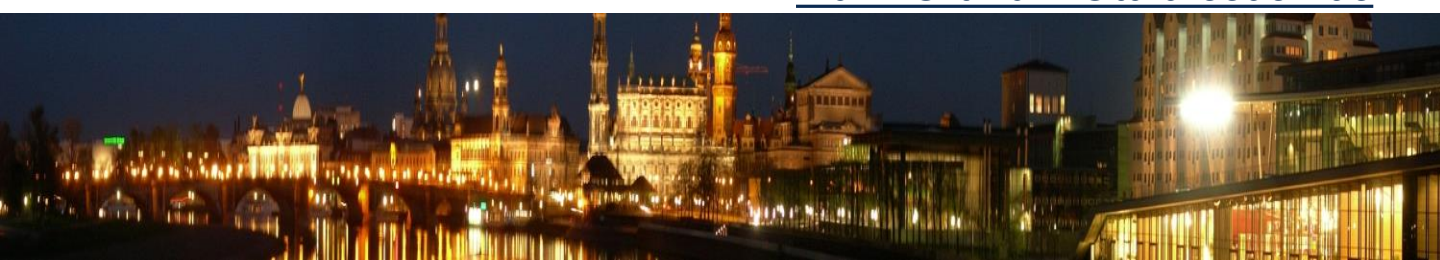

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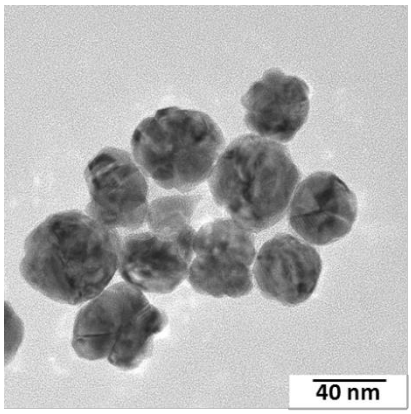
Masterarbeit

Pyroelektrische Materialien für die Desinfektion



Experimentelle Arbeiten zur Funktionalisierung pyroelektrischer Pulver mit Nanopartikeln

Der pyroelektrische Effekt von Materialien wie Bariumtitanat kann genutzt werden, um in wässriger Umgebung OH-Radikale zu erzeugen. Dieser Prozess kann durch Kombination des Pyroelektrikums mit Edelmetall-Nanopartikeln noch verstärkt werden. Im Rahmen der Masterarbeit sollen Palladium-Nanopartikel auf Bariumtitanatpulvern immobilisiert werden und die Generierung von OH-Radikalen mit diesem Material überprüft werden.

Inhalt der Arbeit:

1. Herstellung von Edelmetallclustern in wässriger Lösung
2. Erzeugung von Edelmetallclustern auf der Oberfläche des Pyroelektrikums
3. OH-Radikalnachweis mit dem funktionalisierten Material im Vergleich zu losen Partikeln

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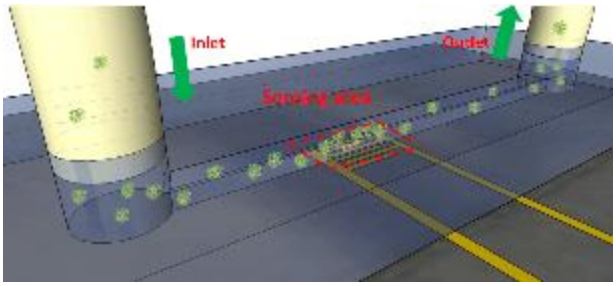
Improvement of sensitivity in field effect transistor biosensors



Specific analyte detection with functionalized field effect transistors

Within a research line at our institute nanomaterials-based field effect transistors (FETs) have been developed for specific analyte detection. In this thesis the aim is to improve their sensitivity by surface chemical modification. To achieve this steps must be followed and characterized. The first part of the work consists on the modification of planar surfaces. The second part includes the transference of the procedure to the FETs and the performance of the detection experiments.

The **research plan** will include:

1.Surface chemistry on planar surfaces and FETs.
2.Analyte detection experiments with FETs
3.Parameter adjustment according to analyzed data

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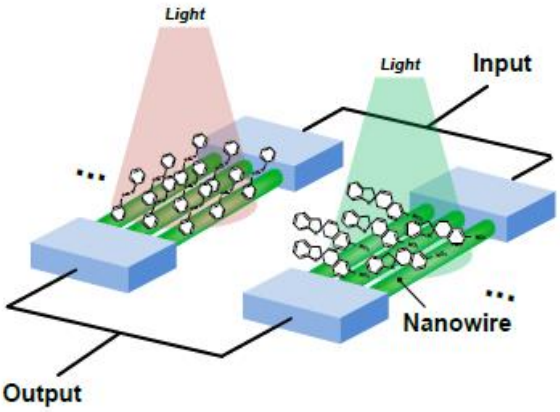
Optoelectronic hybrid nanowire devices

Photoswitching of Si NW FETs using photoswitching molecules



This project aims to develop a fast optoelectronic switching devices using photosensitive molecules. Such molecules, e.g. azobenzenes, diarylethenes or spiropyrans, are highly reactive with light illumination of specific wavelength and change their molecular structure and electrical polarity as a consequence of absorption of photons. Such molecules can be covalently bonded to the oxide surface of Si Nanowire FETs to develop fast switching devices modulated by specific wavelength of light. An important aspect of the project is to find a photoswitching molecule that reveals a fast optical response on a surface.

The **research plan** will include:

1. Surface functionalization of various photoswitching molecules and characterization of the surface (using contact angle measurement, AFM, XPS, FT-IR etc.)
2. Development of optical operating system (LED setup etc.)
3. Electrical characterization of hybrid Si NW FETs

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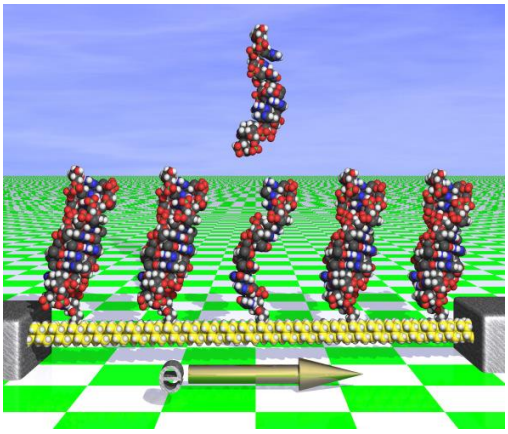

On-Chip Characterisation of One-Dimensional Nanomaterials For Biosensors Application

Semiconducting nanowires and nanotubes integrated in biosensors allow to reach extremely high sensitivity and are able to detect even single molecules or viruses.
The attached charged molecule acts as a gate of a field effect transistor (FET) influencing electronic properties of a nanometer thick conductor. Thus, the electric signals measured with such a FET show the attachment of particular species to the nanowire or the nanotube. The aim of this work is to check and optimize the performance of biosensors based on different one-dimensional materials.

The **research plan** will include:

1.UV-lithography and metalization for fabricating on chip electrodes.
2.Dispersion of one-dimensional nanomaterials on a chip.
3.Electrical investigations of the device performance.
4.Optimization of the device performance by various approaches.

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Photocatalytic reduction of carbon dioxide

Experimental study of reduction properties of CO_2 & simulation

Over the past 30 years, the photocatalytic reduction of carbon dioxide has attracted the attention of many research teams worldwide, and the number of scientific papers on this topic tends to rise. The largest increase was recorded over the past 5 years. However, the scientific community is still waiting for a first economically interesting product.

Here we want to contribute to this field adding new information on the relationship between the optical / electron / textural / structural properties and photocatalytic activity in collaboration with a group from Ostrava. The experimental part will consist in material synthesis, characterization and analytical characterization of the reduction process.

- H.Eckert, M. Bobeth, S. Teixeira, K.Kühn, G.Cuniberti**, Chemical Engineering Journal**, 261 (2015) 67–75.

- K. Kočí, K. Matějů, L. Obalová, S. Krejčíková, Z. Lacný, D. Plachá, L. Čapek, A. Hospodková, O. Šolcová, **Appl. Catal., B** 96 (2010) 239-244.

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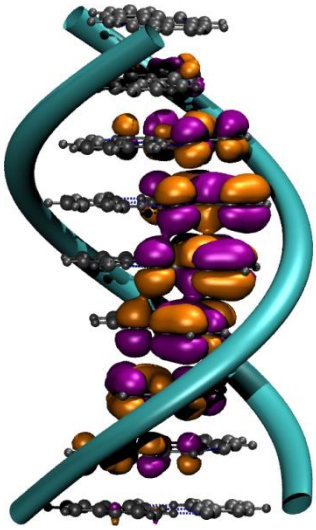
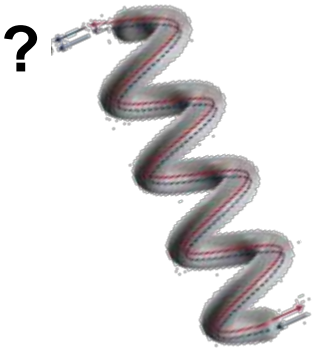


Spin Selective Transport in Helical Molecules

Recent experimental work has shown a strong spin-dependent response in molecular systems like DNA, α–helices, and helicene . This is in so far unexpected as organic systems usually display very weak spin-orbit effects. A common feature to all studied systems is however their **helical** structure. Model-based approaches have suggested a delicate interplay between **helical symmetry** and a non-conventional **spin-orbit coupling**, which could be responsible for the observed spin sensitivity. This chirality-induced spin selectivity can open the door to extensive applications of helical systems in the field of spintronics, thus creating viable alternatives to currently existing semiconductor-based spintronic devices. **Goal** of this Thesis is the formulation of a theoretical framework to describe spin-dependent transport in helical systems both in the coherent and incoherent transport regimes.



The **research plan** will include:

1. Becoming familiar with nanoscale electron transport
2. Learning Master equation techniques
3. Formulation of a model Hamiltonian for helical systems including spin-orbit coupling
4. Numerical solution of the problem and comparison to experiments, whenever possible

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