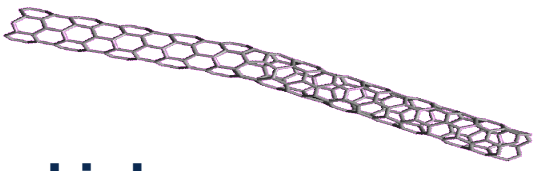
TECHNISCHE UNIVERSITÄT DRESDEN

complex nano materials

2 master theses



Enhancing the electrical properties of horizontally aligned CNTs via introducing kinks

Single-walled carbon nanotubes (SWCNTs) are considered as a promising material for nanoelectronics, because of their excellent electronic and physical properties. Synthesizing SWCNTs with desired electrical properties for nanoscale electronic applications is a main obstacle. In this work, we will try to modify SWCNT by introducing kinks through the growth process and study how this infuences their electrical properties.

research plan for experiments:

1. Establish a well-controlled route for synthesizing horizontally aligned CNT with controlled diameters on different substrates.
2. Establish a well-controlled rotation method for introducing kinks with different angles in the horizontally aligned CNTs.
3. Use atomic force microscopy, raman spectroscopy and scanning electron microscopy in order to characterize the grown CNT.
4. Study the electrical properities of the grown kinked CNTs.

research plan for simulations:

1. Understand the atomic structure of CNTs with kinks.
2. Develop a systematic method to generate the atomic coordinates of such structures.
3. Study the energetic stability of different kinked CNTs.
4. Try to indentify special geometries that can be realized in experiment and eventually lead to new CNT based devices.

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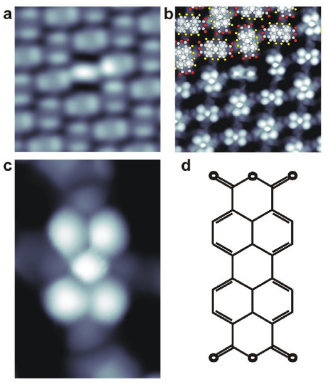
Manipulation of organic molecules by LT-STM

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:

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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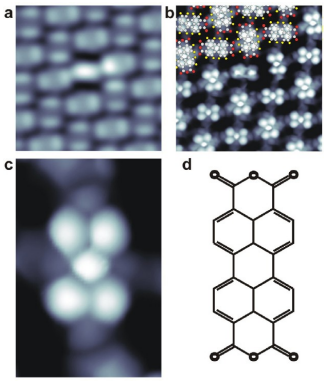
Molecular Blow-up

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



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

Goal of this thesis will be the simulation of STM images of organic molecules (benzene, PTCDA, QTCDA, fullerenes etc.) at metallic surfaces.

The **research plan** will include:

1. Basic understanding of the electronic and structural properties of the relevant metallic surfaces and organic molecules

2. Perform electronic structure calculations and geometry optimizations of the isolated molecules and the molecules chemisorbed (bonded) to metallic surfaces

3. Simulate STM images using DFT combined with Tersoff-Haman approximation

4. Study local heating and destruction of fullerenes under extreme bias voltages

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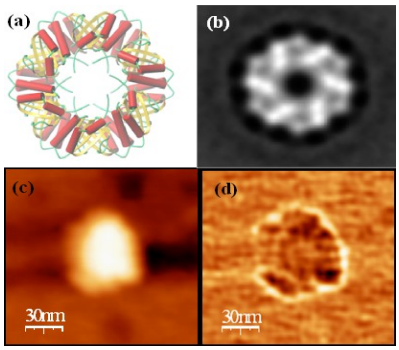
Mechanical properties of SP1 proteins



One of the main challenges of the research within the realm of nano-science and nanotechnology is the ability to form complex combinations of nanomaterials and organize them in a controlled way on surfaces or in forms of wires.
Examples of organized structures can be two-dimensional protein arrays, and hybrids of nanoparticles and bio-molecules, among others. Such structures can be useful for applications ranging from nanoelectronics to medicine. Goals of the thesis are molecular dynamics simulations of SP1 proteins, used in the assembling of quantum dot arrays.

The **research plan** will include:
1. Becoming familiar with the applications of SP1 proteins in nanoelectronics
2. Learning the basics of classical molecular dynamics (MD) simulations of biomolecules
3. Perform MD studies of the dynamics of single and pairs of SP1 proteins and analyze their mechanical stability.

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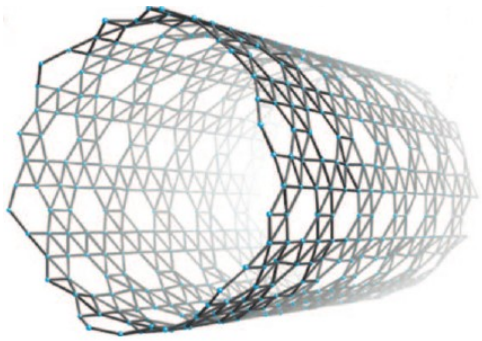
Breathing Nanotubes

theoretical study of vibrations in boron nanotubes



Nanotubes are in the focus of research worldwide. A new and promising material are boron nanotubes and many of its properties still need to be determined. The goal of this thesis is to study the vibrations of boron nanotubes and in particular the so called radial breathing mode. Your results will provide important information that help to understand experimental Raman spectra.

The **research plan** will include:

1. Learning the basics of carbon and boron nanotubes.
2. Understanding the vibrational properties of nanotubes.
3. Getting familiar with continuum mechanics.
4. Developing an analytical description of nanotubular vibrations with continuum mechanics.
5. Learning the basics of density functional theory (DFT).
6. Get introduced to the operation of a DFT code (SIESTA, VASP, DFTB).
7. Performing electronic structure calculations of boron nanotubes and their vibrations.

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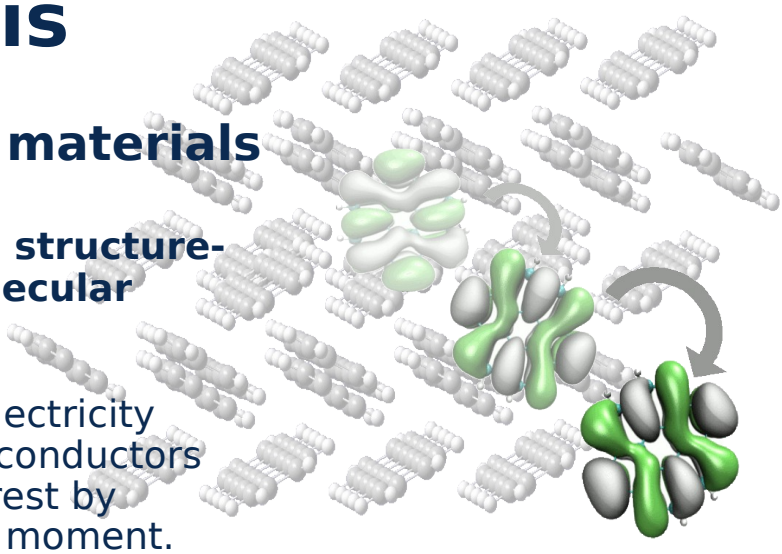
Organic electronic materials

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



Converting sun light into electricity with thin film organic semiconductors is 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.

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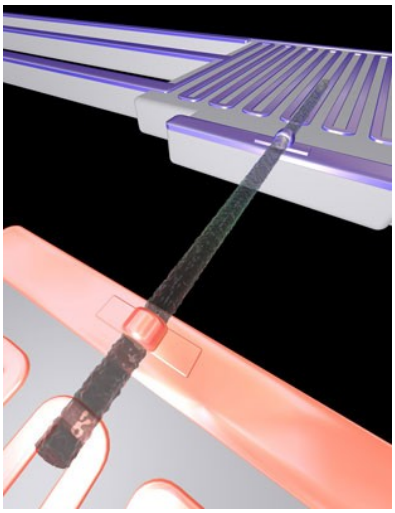

Efficient energy conversion at the molecular level

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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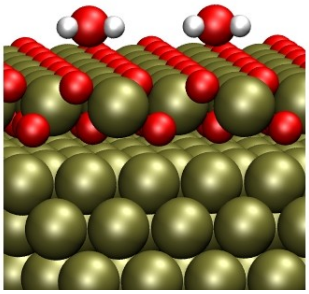
Modeling fuel cells



theoretical study of the adsorption of water on platinum oxides

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.
2. 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).

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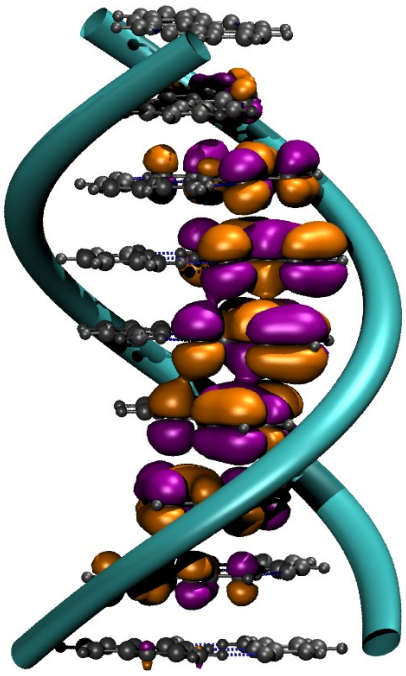
Understanding mutations



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.

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Separation of single walled carbon nanotubes

Single walled carbon nanotubes (SWCNT) have attractive properties for many applications, particularly in the field of electronics like filed effect transistors (FETs). However as-produced SWCNT are always in the bundles including semiconducting and metallic carbon nanotubes, what is the main problem for further applications in electronics.
The project will be related to efficient separation of metallic SWCNT and semiconducting SWCNT from bundled carbon nanotubes. In order to obtain metallic single walled carbon nanotubes separated from the semiconducting.

The **research plan** will include:

1. Preparation of the SWCNT suspension in aqueous solutions.
2. Selective wrapping of SWCNT with DNA or polymers.
3. Sonication of previously prepared solution.
4. Selective oxidation of one type of SWCNT.
5. Electrophoresis processes of defined solutions with SWCNT in agarose gel.
6. Characterization of the separated SWCNT via optical absorption spectroscopy (OAS), Raman spectroscopy and transmission electron microscopy (TEM).

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