<table>
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<tr>
<th>Title</th>
<th>Description</th>
<th>Research group</th>
<th>Contact person</th>
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<tbody>
<tr>
<td>Economic characterization of fusion power plants _part 2</td>
<td>This project intends to further analyze the dependence of economic viability via a range of sensitivity analyses with varying technical and financial assumptions related to both revenue and cost.</td>
<td>Science and Technology of Nuclear Fusion</td>
<td>N.J. Lopes Corzado</td>
</tr>
<tr>
<td>Economic characterization of fusion power plant _part 3</td>
<td>This project will develop and apply learning rate model to capital cost of fusion. Economic data from DEMO2 and PPCS AB will be used to parameterize the model.</td>
<td>Science and Technology of Nuclear Fusion</td>
<td>N.J. Lopes Corzado</td>
</tr>
<tr>
<td>Tailoring nanophotonic structures for optical metrology</td>
<td>The semiconductor industry demands an ever-increasing accuracy in the fabrication of nanostructures. An essential contribution to improved nanofabrication would be the ability to obtain finer information about the produced nanostructures using light. This Bachelor End Project uses concepts from nanophotonics to detect the presence of minute geometrical or material changes. You will simulate the optical response of nanostructures specifically designed for metrology applications. You will use a numerical solver for Maxwell’s equations to predict and quantify the sensitivity of different nanophotonic structures and to optimize the structure design and measurement conditions for robust metrology. The goal is to propose realistic designs to achieve sub-nanometer optical metrology in situations of industrial interest.</td>
<td>Photonics and Semiconductor Nanophysics</td>
<td>A.G. Curto</td>
</tr>
<tr>
<td>Semiconductor nanoantennas for chiral molecular sensing in the ultraviolet</td>
<td>Light gives us information about the chemical and structural composition of matter. Circular dichroism (CD) is one of the most successful and precise optical spectroscopy techniques. It reveals tiny asymmetries in the conformation of nanometric objects of interest like proteins or drugs. CD signals reflect the normalized difference in absorption of a compound when illuminated with light of right- and left-handed circular polarizations. Chiroptical signals are, however, very weak, limiting their potential applications. In this project, you will theoretically investigate the enhancement of chiral light-matter interaction using nanostructures known as optical nanoantennas. The project revolves around numerical simulations. You will design nanophotonic resonators tailored for maximum circular dichroism in the ultraviolet, where chiral biomolecules show their strongest response to circularly polarized light.</td>
<td>Photonics and Semiconductor Nanophysics</td>
<td>A.G. Curto</td>
</tr>
<tr>
<td>Nanophotonics with wide-bandgap van der Waals semiconductors</td>
<td>Van der Waals materials consist of atomically thin layers bound together by weak interlayer forces. A specific subfamily of this class of materials is wide-bandgap semiconductors such as hexagonal boron nitride, which is a highly anisotropic material with an extreme optical response due to strong excitons. You will use a numerical solver for Maxwell’s equations to predict and quantify the nanoscale optical response of different nanophotonic structures. The goal is to enhance light-matter interaction by confining light to deep subwavelength volumes for applications in lithography, photocatalysis, and molecular sensing.</td>
<td>Photonics and Semiconductor Nanophysics</td>
<td>A.G. Curto</td>
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Questions: contact I.M. Kroon
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<tr>
<th>Project Description</th>
<th>Goal</th>
<th>Description</th>
<th>Project Group</th>
<th>Supervisor</th>
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<tbody>
<tr>
<td>Spin-polarized nanophotonics with two-dimensional semiconductors</td>
<td>Atomically thin semiconductors such as monolayer molybdenum disulfide are promising materials for nanoscale optoelectronics and nanophotonics. They also offer access to the spin and valley degrees of freedom as new resources for information technologies. As a bridge between both, circularly polarized light can populate and read out spin polarization. In this project, you will combine the photonic and spintronic properties of nanostructures made of 2D semiconductors. You will use a numerical solver for Maxwell's equations to design nanophotonic resonators for which spin-valley polarization maximally modifies the polarization of light. The goal of the project is to provide a photon-spin interface with enhanced interaction efficiency.</td>
<td>Photonics and Semiconductor Nanophysics</td>
<td>A.G. Curto</td>
<td></td>
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<tr>
<td>Modelling of optical and electrical properties of nanowire solar cell</td>
<td>Goal: Optimize optical/electrical properties of nanowire solar cell towards the increased efficiency. Description: The conversion efficiency of nanowire solar cells highly depends on the nanowire geometry (pitch and shape) and also on electrical properties (charge carrier concentration, p-n junction, and contacts). The goal of this project is to model the optical and/or electrical properties of the full solar cell structure using Lumerical or Comsol software package towards the highest efficiency solar cell.</td>
<td>Advanced Nanomaterials &amp; Devices</td>
<td>J.E.M. Haverkort</td>
<td></td>
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<tr>
<td>Comparison of tapered and inversed tapered nanowires for solar cell applications</td>
<td>Goal: Compare tapered and inversed tapered nanowires for optimized optical properties. Description: In our nanowire solar cells we use tapered nanowires with a smaller top diameter. However, it is not clear if it is better to use conventional tapering or inversed tapering with a bigger diameter on top of the solar cell to have higher open-circuit voltage. The goal of this project is to compare optical properties of both tapered and inversed tapered nanowires to show the optimized structure for the highest open-circuit voltage.</td>
<td>Advanced Nanomaterials &amp; Devices</td>
<td>J.E.M. Haverkort</td>
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<tr>
<td>DFT simulations of perovskites/2D materials heterostructures</td>
<td>Metal halide perovskites (AMX3) have attracted widespread attention over the recent years for their successful application as a semiconductor in high-efficiency solar cells. Due to the flexibility in the choice of the material's constituents (A+ = MA+, EA+, or Cs+; B2+ = Pb2+, Sn2+, X- = I-, Br-, Cl-), the perovskites can show a range of interesting optoelectronic properties. Similarly, two-dimensional materials, which show distinct optoelectronic properties when compared to their bulk counterparts, have attracted lots of attention following the successful isolation of graphene in 2004. Transition metal dichalcogenides monolayers (TMDCs) are an example of a class of atomically thin semiconductors that, like the perovskites, have flexibility in their composition allowing for the tuning of their properties. The aim of this project is to investigate and understand the behavior of heterostructures made from metal halide perovskites and TMDC monolayers. A first step would be the investigation of the properties of the materials themselves using density functional theory (DFT) calculations. When the individual materials are well understood, heterostructures are created and analyzed using DFT calculations as well.</td>
<td>Center for Computational Energy Research</td>
<td>S.X. Tao</td>
<td></td>
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## Alternative Bachelor Final Projects Applied Physics

### DFT simulations of defects in metal halide perovskites

[Defect Physics of Metal Halide Perovskites](https://www.shuxiatao.com/opportunity/bsc-msc-project-4/)

Center for Computational Energy Research  
S.X. Tao

- Defects reduce efficiency loss and lattice degradation
- Study defect concentrations and energy states in order to control them

### DFT simulations of interfaces in perovskite solar cells

[Charge Transport Layers (CTLs) in Perovskite Solar Cells](https://www.shuxiatao.com/opportunity/bsc-msc-project-6/)

Center for Computational Energy Research  
S.X. Tao

- Electron-hole pairs are generated in the perovskite and then separated through the CTLs
- Proper electronic level alignment for optimal charge separation

### DFTB for large-scale simulations of metal halide perovskites

[Our group has been successful in applying Quantum Mechanics (QM) methods, such as, DFT in studying the materials class of metal halide perovskites (18 pristine compounds in total). However, DFT is computationally demanding and often limited to small and pure systems. Simulation of dynamic processes, such as ion migration and degradation reactions in MHP alloys is beyond the capacity of DFT. Classical Molecular Dynamics (CMD) does not suffer from the limitations of DFT and can handle larger systems. However, CMD cannot describe electrons. Consequently, CMD is not suited for studying the chemical reactions and electronic properties of MHP. We meet this challenge in this project by combing the functionalities of describing both electrons and ions in a Semi-empirical QM method, such as, Density Functional Tight Binding method (DFTB).

The goal of this project is to develop new sets of atomic potentials (parameter fitting) dedicated for large-scale simulations (up to 1.000 to 10.000 atoms) of complex metal halide perovskite alloys. We have obtained satisfactory potentials for CsPbI3 and CsPbBr3. A first bachelor/master project will be an extension to other 16 compounds, namely, from Cs to MA to FA, from Pb to Sn, from I/Br to Cl. A second project would be extending the study of pure perovskites to alloys (making the potential parameters transferable), i.e. to simulate CsPb(IxBr1-x)3.](https://www.shuxiatao.com/opportunity/bsc-msc-project-2/)

Center for Computational Energy Research  
S.X. Tao
Alternative Bachelor Final Projects Applied Physics

### Couple dipole modeling of metasurfaces.

In this project, you will develop and implement a coupled dipole model to describe the optical properties of nanophotonic metasurfaces (nanostructured surfaces with unusual properties) that are made of dielectric nanoparticles. The optical resonances of these nanoparticles can be approximated as electric and magnetic dipoles. The dipoles couple with each other due to their interaction through the electric and magnetic field, i.e. the scattering. You will use the coupled dipole model to describe nanophotonic metasurfaces that we are used as cavities for lasing experiments. Another closely related topic to our work that you will investigate will be metasurfaces with bound states in the continuum (BICs). BICs are states that do not suffer losses, i.e. they are resonances with an infinite lifetime. This makes BICs highly interesting for nanophotonic applications.

### Nanophotonics for Solid State Lighting

In collaboration with Lumileds, a multinational leading the market of solid-state lighting, we are investigating different concepts based on nanophotonics for the improvement of LED emission. In this Covid-19 save project, you will be in charge of performing numerical simulations using commercial software that will describe how the emission of LEDs can be modified with metallic and dielectric nanoparticles. The goal of the project is to define different geometries that optimize this emission in two different aspects: the efficiency and the directional outcoupling. The work will be done in close collaboration and with continuous feedback from researchers of Lumileds, to simulate realistic structures that could be fabricated and incorporated in LEDs. Therefore, this research will have a strong applied character.

### Nanophotonic virus sensing

The present COVID-19 pandemic has highlighted the need for fast and economic diagnostic methods which can be applied at the point-of-care and provide an immediate result. Optical biosensing has been widely investigated but has found limited practical use so far, due to the complexity of the involved set-ups. In this project we intend to assess the feasibility of optical sensing of viruses using nanophotonic structures and simple optical read-out methods. Photonic crystals and plasmonic structures, defined by nanoscale patterning, define a spectral resonance, whose frequency depends on the dielectric environment. By functionalizing the surface with proper bioreceptors, target biological molecules such as antibodies or even viruses can be selectively trapped on the surface. This changes the refractive index and thereby the resonant frequency and can be detected optically (see figure). The goals of this project are:

- Calculate (using commercial electromagnetic simulation software) the reflection spectra of extended photonic crystal structures and the wavelength shifts due to a thin layer of biological molecules (antibodies) trapped to the surface
- Calculate the reflection spectra of localized photonic crystal structures and the wavelength shifts due to a single virus trapped at one location. If time allows: Compare the results with confined plasmonic structures
- Propose a practical sensing configuration for antibody/virus detection, employing low-cost optical components.

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Photonics and Semiconductor Nanophysics  
J. Gómez Rivas

Photonics and Semiconductor Nanophysics  
J. Gómez Rivas

Photonics and Semiconductor Nanophysics  
A. Fiore
### Design of a fiber-coupled nanophotonic sensor

Photonic crystals are nanophotonic structures based on a periodic modulation of the refractive index. They allow defining sharp spectral resonances whose wavelength depends on the environment (temperature, refractive index, force, etc), making them exquisite optical sensors. Our group is exploring photonic crystal sensors placed on the tip of optical fibers and optimized for read-out via the fiber, e.g. for application in refractive index sensing (see figure). In this project, you will explore the optical properties of these structures and their design. Nanophotonic cavities have so far been designed for the strongest light confinement, low loss and in some cases optimal coupling to a waveguide. Here we want to tackle a new challenge: how to design a cavity which confines light on a submicrometer length scale while efficiently coupling the radiated field into an optical fiber – without any external lens. You will make use of advanced concepts in photonic crystal design and a commercial electromagnetic simulation software to devise new structures for sensing. The goal is to find a structure which confines the electromagnetic field to the smallest possible region with low loss, while producing a clear spectral feature in the reflection spectrum. The resulting designs will be tested experimentally in our group (though this not be part of the project).

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<th>A. Fiore</th>
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#### Optimization of the optical properties of a multi-pixel array for spectral sensing

Optical spectroscopy is widely used for the classification of materials and quantification of their biochemical properties, particularly in the agro-food sector (e.g. to measure ripeness of fruit, predict taste, etc.). The problem is that the traditional spectrometers expensive and bulky, which limits their use to laboratories and industry. To make spectroscopy available for a larger range of applications there is a growing trend in miniaturizing these devices. In this project we want to optimize the optical response of our developed micro-spectrometer operating in the Near-Infrared region (840-1700 nm) for specific applications. The micro-spectrometer is made of an array of resonant cavity-enhanced photodetectors, where every pixel has a different wavelength response (Fig. a). In this approach every pixel contains an active area which absorbs the incoming light together which is co-integrated with a filter inside a cavity. A sketch of a single pixel is shown in Fig. b, where the tuning element and the active InGaAs/InP layers are placed inside the cavity formed by the Au and Ag mirror. The optical response of the cavity is controlled by changing the thickness of the tuning layer (Fig. c). Currently we have shown that we can fabricate these micro-spectrometers and perform spectral sensing. An example of this is the optical measurement of tomatoes with different sugar content. Fig. d shows the measured photoresponse of 15 used pixels for different tomatoes (indicated by the different sugar levels). Compressive sensing algorithms are used to obtain the interesting properties like sugar from the photocurrent values. The quality of the strongly depends on the optical response of our cavity structures. The goal of this project is therefore to optimize the structure using Finite Difference Time Domain (FDTD) simulations. The influence of several of those structure parameters (e.g. the thickness and position of the absorbing layer) on the optical response will be investigated. It is important to understand how these will influence physical properties like the FWHM of the modes, the maximum absorption, the peak wavelengths, field distributions etc. It is also interesting to investigate the relation between the resonant wavelengths and the ability to determine a certain property like sugar or fat in e.g. milk using already available data sets. This will drive the design of new generations of spectral sensors.

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**Figure:** (left) Concept of fiber-tip sensor; (middle) Electron microscope image of a sensor fabricated at TU/e; (right) Reflection spectra when the sensor is immersed in two different liquids.

**Figure:** a) and b): Schematics of the sensor array; c) Calculated spectral responses for the different pixels; d) Measured photocurrents for different tomatoes.
<table>
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<tr>
<th>Project Title</th>
<th>Description</th>
<th>Theory of Polymers and Soft Matter</th>
<th>Faculty Member</th>
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<tbody>
<tr>
<td>Structural correlations in glass-forming materials</td>
<td>Understanding the liquid-to-glass transition ranks among the deepest unsolved problems in physics. All existing (incomplete) first-principles theories of the glass transition assume that the structural properties of a glass-forming material can be described by simple correlation functions, but it is very plausible that more intricate (high-order) structural correlations should be considered. The goal of this project is to extract these high-order structural correlations from our simulation data.</td>
<td>L.M.C. Janssen</td>
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<tr>
<td>Double ring-polymer networks</td>
<td>A method developed in our group to generate random space-filling configurations of ring polymers may provide a novel way to create double network elastomers (super-tough rubber-like materials) entirely out of intertwined rings. Simulations will tell us how well this works.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>W.G. Ellenbroek</td>
</tr>
<tr>
<td>Novel polyelectrolyte membranes for flow and fuel cells</td>
<td>Atomistic molecular-dynamics computer simulations of Nafion/graphene oxide nanocomposites using Gromacs and LAMMPS software packages. The goal is the connection between the heterogeneous structure and the details of the proton transport in these devices.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>A.V. Lyulin</td>
</tr>
<tr>
<td>Catch a killer</td>
<td>Using molecular dynamics simulations, we generate data for large systems of mostly randomly moving particles (&quot;people&quot;) enriched with one or more &quot;assassins&quot;; particles that are differentially attracted to one specific other random particle, whose location they always know. Now, what if we pretend we don't know anything about these data. How hard is it to identify the assassins and their victims in large data sets for different attractive potentials? How about if we incorporate more realistic crowd dynamics?</td>
<td>Theory of Polymers and Soft Matter</td>
<td>C. Storm</td>
</tr>
<tr>
<td>Supramolecular polymers of cyclodextrins and DNA</td>
<td>Theory of reversible assembly of cyclodextrins and short pieces of DNA into long tube-like fibres for gene therapy, and explain why the assembly is so strongly co-operative. Statistical mechanics of the Tonks gas, in combination with mass action theory.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>P.P.A.M. van der Schoot</td>
</tr>
<tr>
<td>Spin glasses</td>
<td>Spin glasses are a variant of the Ising model, and they provide excellent model systems to study the physics of glass formation. The goal of this project is to derive and/or numerically simulate the glassy dynamics of one specific family of spin-glass models; the results will provide a benchmark for existing theories of the glass transition.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>L.M.C. Janssen</td>
</tr>
<tr>
<td>Monte Carlo simulations of constrained polymers</td>
<td>Monte Carlo simulations of polymeric materials are nontrivial because many polymer models involve hard constraints on bond lengths and bond angles. We will explore new ways to do this, and apply these to semiflexible polymers, small-scale network models, or the rotational isomeric state model (an atom-scale model for simple hydrocarbon chains).</td>
<td>Theory of Polymers and Soft Matter</td>
<td>W.G. Ellenbroek</td>
</tr>
<tr>
<td>Novel phase change materials for optimal thermal energy storage</td>
<td>Atomistic molecular-dynamics computer simulations of paraffine/CNT/graphene nanocomposites using Gromacs and/or LAMMPS software packages. The goal is to provide insights into the mechanisms of the (still) very low thermal conductivity in these amorphous compounds.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>A.V. Lyulin</td>
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<td>Title</td>
<td>Description</td>
<td>Supervisor</td>
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<tr>
<td><strong>Influence of collisions on ALD</strong></td>
<td>Atomic layer deposition (ALD) is a technique to deposit thin layers on a substrate with atomic precision in the vertical direction. In ALD precursors are added to the system and these can react with the substrate, the probability of reacting is determined by the temperature, the reaction energy and the time spent near the surface of the substrate. The time spent near the surface depends on the van der Waals interaction between the precursor and the substrate but also on collisions with other precursors and reacted particles on the substrate. The student will study by molecular dynamics simulations the influence of collisions on the time spent of precursors near a surface.</td>
<td>Theory of Polymers and Soft Matter</td>
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<tr>
<td><strong>Physics of membraneless cell organelles</strong></td>
<td>Model organelles of oppositely charged polymeric molecules: internal structure, interactions with proteins, role of charge distributions and size. Specific focus is on the structure of the complexes near embedded model proteins, the role of excluded volume interactions. Analytical, numerical and simulation projects are possible, the latter with the LAMMPS package.</td>
<td>Theory of Polymers and Soft Matter</td>
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<tr>
<td><strong>Active matter</strong></td>
<td>So-called active particles can become self-propelled by a chemical gradient. Here you will explore how such particles respond to a point source of chemical fuel, with the aim to mimic sensing and self-organizing behaviour of living systems. The results can be compared with ongoing experiments by Prof. Jan van Hest and Dr. Loai Abdelmohsen (Chemistry department). Simulations in Fortran 90, data analysis in favorite programming language.</td>
<td>Theory of Polymers and Soft Matter</td>
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<tr>
<td><strong>Identifying novel crystal structures in colloidal systems</strong></td>
<td>Hairy colloids are promising candidates for making unusual crystals with symmetries that hard to make otherwise – or even entirely novel. We have simulation data (real-space structures) and experimentally obtained X-ray diffraction patterns. How can we combine these to tell a story?</td>
<td>Theory of Polymers and Soft Matter</td>
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<tr>
<td><strong>Glassy structure and segmental mobility in free-standing thin polymer films</strong></td>
<td>Atomistic molecular dynamics computer simulations of dense polymers in thin films in absence of a substrate using an in-house developed software package.</td>
<td>Theory of Polymers and Soft Matter</td>
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<tr>
<td><strong>Dynamics of cancer cells</strong></td>
<td>Recent in-vitro experiments by Dr. Vito Conte (BME department) indicate that cancer cells are much more mobile than healthy cells. The cell dynamics of the cancer cells also appears to be fundamentally different, but the physical processes at play are still poorly understood. This project aims to shed more light on the physics of the experimental cancer-cell dynamics, using data analysis tools and/or computer simulations.</td>
<td>Theory of Polymers and Soft Matter</td>
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<tr>
<td><strong>Donnan theory of charge accumulation in viruses</strong></td>
<td>Viruses and other protein shells are characterised by the presence of large numbers of charges that are either fixed to the inner surface of the shells or fixed to cargo molecules held within these shells. This leads to a redistribution of small ionic species between the shell and the bulk solution that in turn leads, e.g., to significant shifts of the acidity and ionic strength. In the project, Donnan theory will be applied to cargo molecules with weakly ionic moieties to investigate shifts in degree of ionisation.</td>
<td>Theory of Polymers and Soft Matter</td>
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<td><strong>Code development for active particles</strong></td>
<td>Large-scale particle-based computer simulations can be performed very efficiently using (open-source) simulation packages such as LAMMPS. However, we do not yet have a LAMMPS implementation for active particles. In this project you will develop and modify the LAMMPS code to realize such active-particle simulations. For testing purposes, we can compare the LAMMPS results with our home-built code. If successful, we will use the new LAMMPS code in several PhD studies. Strong affinity with programming (in particular C/C++) is definitely a must!</td>
<td>Theory of Polymers and Soft Matter</td>
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<td>Project Title</td>
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<td>Group Name</td>
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<tr>
<td>(In)homogeneities in tetraPEG gels</td>
<td>TetraPEG gels are polymeric hydrogels made from 4-arm star polymers, that have been claimed to be much more spatially homogeneous that typical polymeric gels. We wish to investigate this claim numerically. How homogeneous are they, really?</td>
<td>Theory of Polymers and Soft Matter</td>
<td>W.G. Ellenbroek</td>
</tr>
<tr>
<td>Molecular dynamics of multilayer single polymer films</td>
<td>In this project we undertake multiscale simulations of semi-crystalline morphology development upon high strain mechanical deformation of polyethylene and polypropylene to understand the mechanisms controlling crystallization, toughness, permeability, determine optimization design strategies and provide a molecular basis for finite-element simulations.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>A.V. Lyulin</td>
</tr>
<tr>
<td>Stretching Chromosomes</td>
<td>During mitosis, DNA is condensed into a tightly packed form called the mitotic chromosomes: thick cylindrical structures that allow for accurate division of the genetic material between the daughter cells. Precisely how this iconic form is organized remains unknown, but it is clear that helper proteins called condensins and topoisomerases play an important role. The research team of prof Wuite at the VU in Amsterdam is doing experiments in which this complex hierarchical structure is slowly pulled apart, like the unraveling of knitwork. We will use continuum models and polymer physics to infer what such experiments can teach us about the organization of mitotic chromosomes.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>C. Storm</td>
</tr>
<tr>
<td>Dispersions of concentrated rod-like viruses</td>
<td>Solving the inhomogeneous Onsager equation for the isotropic-nematic transition of bidisperse rod-shaped particles, and calculate the interfacial tension between isotropic and uniaxial nematic liquid-crystalline phases. Numerical and analytical projects are possible.</td>
<td>Theory of Polymers and Soft Matter</td>
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<tr>
<td>Collapse in soft particle packings</td>
<td>Excessive pressure load on a material often leads to structural collapse. The same is true if the material is composed of a mixture of soft particles tightly packed together. In this project you will develop and use a new code to identify the optimal strategies to increase the stability of soft particle packings under pressure. Programming in C/C++.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>S. Ciarella</td>
</tr>
<tr>
<td>Optimizing the performance of filler particles for bioplastics</td>
<td>Hard rod-shaped particles can greatly improve the strength and stiffness of plastics, but only if they mix well with the polymers. Can we improve this mixing by modifying the surface of the fillers?</td>
<td>Theory of Polymers and Soft Matter</td>
<td>W.G. Ellenbroek</td>
</tr>
<tr>
<td>Collagen deposition in drying droplets</td>
<td>Coffee stains are the result of the evaporation of a droplet containing dissolved solids. As the stains show, the solid is deposited on the surface non-uniformly. Something similar happens when a droplet containing the biopolymer collagen evaporates. The long thin strands of collagen are deposited on the surface in fascinating patterns, switching between radial, concentric and random. The resulting micropatterns are not just beautiful to look at – cells sense the changing orientations and respond to them. In this project, we theoretically investigate the coupling between flow, polymer orientation and substrate deposition to understand and predict the patterns.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>C. Storm</td>
</tr>
<tr>
<td>Shape of droplets in narrow non-wetting tubes.</td>
<td>Droplets in immiscible fluids confined to non-wetting capillaries usually have the shape of a sphere or an end-capped cylinder, but in some cases they resemble a groundnut. In order to investigate why, we set up a variational theory for the shape of a drop confined in a radially symmetric repulsive potential.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>P.P.A.M. van der Schoot</td>
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Effective interactions between hairy colloids

Particles that interact with so-called shoulder potentials have been widely reported numerically to be able to show quasi-crystalline phases. The most commonly proposed way to realize such potentials is with hairy colloids. Let us use simulations to figure out what these colloids should look like to actually make quasicrystals.

Mechanics of vacumated EPS granules

Expanded polystyrene or EPS is an important packaging and construction material, famed for its low density and excellent thermal isolation qualities. At the microscale, individual EPS granules (or ‘pearls’) are cellular solids with thin walls that separate large voids; the material is mostly air. With an industrial partner, we are interested in the options for compacting it for more efficient transport. You will model the response of single and packed pearls to various degrees of evacuation using the simulation package COMSOL, and will conduct simple mechanical tests to validate the results.

Fracture microscopics: does the measurement affect the outcome?

A way to assess where chemical bonds are breaking in a disordered material is including molecular units that become fluorescent when they break. But if these units are of a different strength than the rest of the material, the fracture properties of the material might change due to their addition. We will develop analytic and/or numerical models to assess whether this happens.

Stiffening polymer gels with active particles

Many biological and polymeric materials stiffen when they are deformed. This nonlinear elasticity provides important functionalities, as it may protect materials from becoming damaged by limiting the strains at high loading. Experiments in Eindhoven are investigating the possibility of applying the stiffening stresses from within, by infusing a polymer material with active particles that actuate the solvent. The resulting hydrodynamic stresses may act as triggers for stiffening, creating a material whose stiffness may be externally controlled without the need for deformation. In this project, you combine polymer theory, active matter theory, and mechanical modeling to understand and predict this effect.
### Simulation-based design of meta-lenses for controlling optical fiber output

Optical fibers are the backbone of modern communication infrastructure and the focus of intensive research. In the PSN group, we use their attractive properties for other areas such as optical sensing. Recently, we have developed a new method for efficiently mass-producing photonic structures on fiber-tips. The process has so far been demonstrated for creating optical sensors suitable for the detection of a range of stimuli such as temperature and refractive index (fig a). Optical fibers are the backbone of modern communication infrastructure and the focus of intensive research. In the PSN group, we use their attractive properties for other areas such as optical sensing. Recently, we have developed a new method for efficiently mass-producing photonic structures on fiber-tips. The process has so far been demonstrated for creating optical sensors suitable for the detection of a range of stimuli such as temperature and refractive index (fig a). As a next step in this line of research, we want to investigate ways of using our technique to tailor the properties of the light emitted from the fiber. This will be achieved using meta-lenses, lenses based on sub-wavelength engineered structures, allowing their capabilities to go beyond those of a conventional lens (fig b). The project focuses on the design of a meta-lens for focusing the light from a standard single-mode fiber to an elliptical profile matching standard semiconductor lasers. This result is reached through a number of intermediate steps:

- A meta-lens consists of a large number of resonant elements (see fig b); a first step is simulating the interaction of a single resonator with the surrounding electromagnetic field.
- Once the characteristics of a single element are known, ensembles of elements are simulated to create the desired focusing effect, completing the meta-lens.
- Finally, the interaction of the lens and the optical fiber is simulated to validate the full structure.

### How does confinement shift the phase transitions of a crystal

Crystal hydrates are a promising class of materials for long term thermal energy storage. Cyclic hydration/dehydration reactions involve large rearrangements of the crystal structure, which can lead to disintegration of the material. Therefore, stabilization methods are needed. A form of stabilization is confinement of the crystal in a mesoporous material. The question is how the phase transitions respond on the confinement. Two particular phase transitions can occur: the hydration/dehydration reaction itself and deliquescence (the crystal dissolves by absorbing water vapor). Objective and approach: Develop a thermodynamic model able to predict the shift of the phase transitions due to confining the crystal. The model has to make a connection between the temperature and water vapor pressure at which the phase transitions occur and properties of the crystal.

### Thin water films on surface of extremely soluble surfaces

Crystal hydrates are a promising class of materials for long term thermal energy storage. The storage principle is based on a hydration reaction: a crystal absorbs water in its crystal lattice. There are indications that water films at the crystal surface facilitate this process. Presently little is now about water films on this type of surfaces. The question is how the thickness of a water film on a surface of an extremely soluble salt varies with the water vapor pressure. We expect that dissolved ions stabilize thick water films. Objective and approach: Develop a “disjoining pressure type of model” to predict the thickness of a water films as a function of the applied water vapor pressure and the solubility of a crystal. As the topic deals with extremely soluble salts, special attention has to be paid the description of water/ion film.
### Alternative Bachelor Final Projects Applied Physics

<table>
<thead>
<tr>
<th>Project Title</th>
<th>Description</th>
<th>Objective and Approach</th>
<th>Author(s)</th>
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<tbody>
<tr>
<td>Reaction of a particle in a 2D storage device</td>
<td>Crystal hydrates are a promising class of materials for long term thermal energy storage. To use them in a storage device salt hydrate powder is compressed to tablets. In the device water vapor is blown along the tablets that react by hydrating. Presently we are constructing a 2D device for studying the behavior of particles during hydration/dehydration cycles. The question is: can we model the flow, vapor diffusion around and reaction with a spherical particle?</td>
<td>To model the flow, vapor diffusion around and reaction with a spherical particle</td>
<td>H.P. Huinink</td>
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<td>Forces between suspended particles in Magnetic Density Separation</td>
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<td>t.b.a.</td>
<td>A.A. Darhuber</td>
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<tr>
<td>Manipulation of thin liquid films with surface charge patterns</td>
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<tr>
<td>Moving matter with light: flows induced by photochemical reactions</td>
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<td>t.b.a.</td>
<td>A.A. Darhuber</td>
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<tr>
<td>Surface functionalization using small inhibitor molecules for area-selective atomic layer deposition</td>
<td>To enable further downscaling of electronics, self-aligned fabrication schemes are required to relieve some of the alignment constraints that are currently the bottleneck for advancement in the semiconductor industry. For this reason, area-selective ALD is gaining interest since it could play a vital role in self-aligned fabrication. The aim of area-selective ALD is to deposit material only where required as opposed to currently employed techniques which rely on lithography and etching. Our recently developed approach to area-selective ALD relies on the use of small inhibitor molecules dosed in vapor-phase in three step ALD cycles.</td>
<td>To make a selection of molecules that would be interesting as inhibitor for area-selective ALD. Since the use of inhibitor molecules for area-selective ALD is a relatively new concept, the study will challenge you to think outside of the box and puzzle together information from other fields of literature.</td>
<td>A.J.M. Mackus</td>
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<tr>
<td>Studying plasma atomic layer etching applications in fabrication of AlGaN/GaN RF and high electron mobility transistor devices</td>
<td>Atomic layer etching (ALE) is set to become one of the key processes for further downscaling of integrated circuits (IC) because of its high level of etch control, smoothing effect and selectivity to the desired etched material. Current Si based high power and high frequency communication devices are running up against the theoretical limit of scaling and performance. To continue the pursuit of better communications devices, new materials will have to be leveraged. One such material being considered for this application is AlGaN/GaN. When these materials are stacked together, a 2D electron gas (2DEG) is formed at the interface, the presence of which imparts a high carrier concentration as well as a high electron velocity within the channel region of the device. The fabrication process for these devices involves reactive ion etching, however this is hard to control and can often leave a damaged etch front which ultimately degrades device performance. In this project, the student will unravel the fabrication process of normally-off AlGaN/GaN based devices, and identify key steps within the fabrication process that could be replaced by an ALE step to enhance device performance. By studying scientific and patent literature new application possibilities will be identified</td>
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<td>A.J.M. Mackus</td>
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<td>Project Title</td>
<td>Description</td>
<td>Relevant Field</td>
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<td>Area-selective atomic layer deposition for fabrication of nanodevices</td>
<td>The continuous down-scaling of the semiconductor devices has led to a drastic increase in the manufacturing cost and process complexity. Therefore, an area-selective deposition method is desired to deposit materials only where it is needed and to minimize the number of required processing steps. An area-selective ALD method has been recently developed by sequentially dosing inhibitor, precursor and coreactant gases, where the introduction of inhibitor molecules plays an important role in determining area-selectivity of the growth process. In this project, you will perform stochastic simulations on candidate inhibitor molecules to study the influence of molecule size, shape and substrate lattice parameters on its blocking ability. With these stochastic simulations, you will identify inhibitor molecules that can adsorb with a high packing on a surface.</td>
<td>Alternative Bachelor Final Projects Applied Physics</td>
<td>A.J.M. Mackus</td>
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<td>Theoretical study of micrometer particle levitation in a plasma environment.</td>
<td>Creating a plasma is relatively easy: take a low pressure gas vessel, put a sinusoidal voltage at radio frequency on a metal plate in the vessel and a plasma is made. This will create a beautiful plasma-discharge, which can be used in various high tech applications. However, exact knowledge of how the fundamental processes take place at the edge of the plasma is hard to obtain. Traditional methods of measuring the relevant processes cannot be applied to the edge of the plasma. A different method is to use a single microparticle as a probe, which can levitate in the edge of the plasma because the several plasma-induced forces working on the particle cancel each other out. One of the forces which makes levitation possible, is the thermophoretic force. This force comes from the difference in momentum transfer by hot and cold gas particles striking the dust particle from different sides. This will cause the particle to experience a net force, anti-parallel to temperature gradient. It will be your job to analyze the relevant plasma- and temperature gradient induced forces working on the particle and implement these in a semi-analytical model. This model could shed new light on currently not understood issues such as hysteresis in the force balance, shown by the particle under varying hypergravity conditions.</td>
<td>Plasma &amp; Materials Processing</td>
<td>P. Meijsaard</td>
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<td>The swelling kinetics of hydrogel fibers</td>
<td>Hydrogel systems have gained significant interest for biomedical applications such as drug delivery, tissue engineering or soft robotics. Recently, 3D-printed supramolecular hydrogel fibers showed reversible transformation upon swelling and deswelling to act as a shape-morphing system. The dimensional change of the 3D-printed fiber during swelling, has been mapped in detail. However, the kinetics of the hydrogel has not been understood in order to predict the swelling behavior for different dimensions. The aim of this project is to study the physics of the supramolecular hydrogel fibers during aqueous transformation in order to build shape-morphing systems in various the shape and dimension.</td>
<td>Theory of Polymers and Soft Matter</td>
<td>C. Storm</td>
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<td>Particle Swarm Optimization of the Near-field Produced by Nanoparticle Arrays</td>
<td>A significant scientific effort has been made over the past few decades in controlling and enhancing the optical response of metallic nanoparticle arrays. The nanoparticles in periodic arrays support collective resonances which originate from the radiative coupling of localized resonances in the individual nanoparticles, giving rise to very strong and spectrally narrow optical responses. The strong optical response produced by lattice resonances is usually reflected in the far-field behavior of the array, resulting in large values of extinction. However, this is not consistent with near-field response of the array, for example, the electric field is also increased by the excitation of a lattice resonance, but is not bounded and could be enhanced arbitrarily in principle. Therefore, there are two questions arise: (1) What is the strongest enhancement of the near-field that a surface lattice resonance (SLR) can produce?</td>
<td>Photonics and Semiconductor Nanophysics</td>
<td>J. Gómez Rivas</td>
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**Alternative Bachelor Final Projects Applied Physics**

(2) Under which geometrical parameters of nanoparticle arrays can this field enhancement be achieved?

In this project, Particle Swarm Optimization (PSO) algorithm can be employed to obtain the largest enhancement of near-field by optimizing the geometrical dimensions of plasmonic arrays (periodicity of array, height and diameter of nanoparticles). In a recent paper [1], the authors show that, as the near-field enhancement increases, the length scale over which it extends above and below the array becomes larger. So the third question arise:

(3) What is the largest decay confinement length perpendicular to the plane of array and what is the largest propagation length in this plane?

In this work, we will investigate the relationship between the near-field enhancement and different length scales of the system in and perpendicular to the array plane. This work will provide a valuable understanding of the near-field produced by the lattice resonances of periodic arrays of nanoparticles, and therefore will serve to guide experimental efforts seeking to exploit the extraordinary optical response of these systems.


<table>
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<tr>
<th>Optimal Nanoparticle Arrays for Net Enhancement of Photogeneration Rate in Organic Solar Cells</th>
<th>Photonics and Semiconductor Nanophysics</th>
<th>J. Gómez Rivas</th>
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<td>Organic solar cells (OSC) have gained much attention in the last decade due to their advantages such as low-cost, ease-of-fabrication, flexibility, light-weight as well as tunability of their properties. However, the lower performance of OSCs compared to inorganic solar cells can be attributed to poor charge transport properties and high charge recombination rate in the active organic layer, limiting the optimum layer thickness for light absorption. Due to the low charge carrier mobility and high recombination rate in OSCs, charge collection efficiency will be very poor if the active film of OSCs is too thick. On the other hand, if the active layer is too thin, most of the sunlight will not be absorbed to create charges. To address these issues, further research focusing on improving light absorption and reducing recombination in organic solar cells is needed. Towards this goal, one possibility would be to design and synthesize new organic materials. Another promising approach is to employ light trapping strategies on existing material systems. Light trapping allows the active layer to absorb more of the light, while keeping the thickness thin enough for charge extraction. The incorporation of resonant nanostructures into organic solar cells offers an attractive light trapping and absorption approach to enhance the power conversion efficiencies. In this project, metallic or dielectric nanoparticle arrays will be investigated to increase the light absorption in OSCs. Numerical simulations based on the FDTD method and Particle Swarm Optimization (PSO) algorithm will be used to optimize the optical enhancement in solar cells and improve the performance of OSCS devices.</td>
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<th>A molecular model of nanoparticle receptor targeting</th>
<th>Theory of Polymers and Soft Matter</th>
<th>C. Storm</th>
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<td>Target drug delivery is based on the use of nanoparticles (1-100 nm in size) as drug carriers able to selectively address medicine to the correct site (e.g. delivering anti-cancer drug only to the tumor tissue). This is achieved by molecular recognition of cell membrane receptors that are expressed specifically on the surface of diseased cells. However, the design of such system is incredibly complex as many variables have to be taken in account namely the particle size, the number, distribution and affinity of the targeting ligands on the nanoparticles and the amount and mobility of the receptors on the cell. A quantitative understanding of the impact of such parameters is therefore important for the design of the next generation of drug delivery carriers. In this project a coarse-grained molecular model will be built to dissect the contribution of the different structural parameters and to predict the properties of the ideal drug carrier.</td>
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