Forslag til Prosjektoppgaver, høsten 2018
Forslag til Masteroppgaver, våren 2019

# TKT4540 - Nanoteknologi, fordypningsprosjekt
# TKT4930 - Nanoteknologi, masteroppgave

NTNU Nanomechanical Lab
www.ntnu.no/nml

Veileder:

Professor Jianying He

Professor Zhiliang Zhang

Group introduction:

**NTNU Nanomechanical Lab** (NML) was established in 2006 as part of the NTNU Nanotechnology. Currently there are 2 permanent faculty members, **Professor Zhiliang Zhang** who is on sabbatical leave at California Institute of Technology until June 2018, and **Professor Jianying He,** 17 PhD students and 3 postdoc research fellows in the group. 5 of the PhD students are from MTNANO program in addition to 1 from MTNANO already finished his PhD. In the past, NML has supervised 9 master students in Nanotechnology. In addition to other ongoing projects, Prof. Zhang and Prof. He are both leading so-called FRINATEK (hard competition) projects financed by the Research Council of Norway.

Our research focuses on both the fundamental understanding of the nanoscale mechanisms and applied nanotechnology. The topics varied with nanostructured materials and surfaces for anti-icing, effective $CO_2$ condensation, thermal interfacial material enhanced heat transfer, nanoscale additive manufacturing et al. Both atomistic simulations (density functional theory and molecular dynamics) and synthetization, fabrication and characterization using NTNU NanoLab and NML.

Our recent research news:
**Får problematisk is til å sprekke opp**
**Den brennende isens hemmeligheter**

Our latest research paper appeared in the ***Nano Letters***:
**Grain-size Controlled Mechanical Properties of Polycrystalline Monolayer $MoS_2$**

**List of topics:**

- Super-Dewetting Surfaces
- Super-Low Ice Adhesion Surfaces
- 3D Printing of Nano-Architected Metals
- Real-Time Molecular Dynamics Simulation for Nano-Engineering Energy Storage Materials
- Discover $CO_2$-phillic materials by Deep learning
- Wetting on 2D single-layer molybdenum disulfide $MoS_2$
- Syntheses and Multiphysical Characterization of Ultra-thin Metal Film on Polymer Substrate

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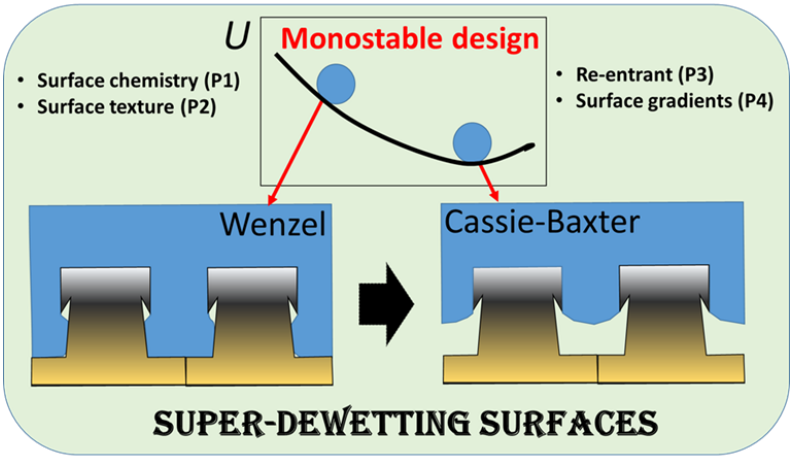
|---|---|
| **Title** | **Super-Dewetting Surfaces** |
| **Supervising team** | Professor Zhiliang Zhang, zhiliang.zhang@ntnu.no<br>Professor Jianying He, jianying.he@ntnu.no<br>www.ntnu.no/nml |
| **Background** | In the past decade we have witnessed a drastic increase in the understanding and applications of the so-called superhydrophobic surfaces. It is now well understood that a superhydrophobic surface with its ability to repel invading water—that is, to display a very large apparent contact angle (> 150°) and a very small roll-off angle, can be created by combining the surface roughness with a hydrophobic material. Superhydrophobic surfaces find numerous applications, for example, in oil-water separation, drag reduction, stain repellency, self-cleaning, fog harvesting, micro fluidics and efficient dropwise $CO_2$ condensation. However, the development of the state-of-the-art superhydrophobic surfaces has come across one bottleneck. Surface superhydrophobicity is attributed to the formation of the Cassie-Baxter wetting state where a water droplet contacts only the tips of the rough surface. The problem is that the designed Cassie-Baxter state is mostly metastable. The superhydrophobicity is remarkably fragile and can break down, due to the wetting of the surface texture to yield the Wenzel state under various environmental conditions, such as elevated pressure, high droplet impact and in particular vapor condensation. Due to large energetic barriers that impede the reverse transition (dewetting), this breakdown in superhydrophobicity has been widely believed to be irreversible.<br>Recently, there is a clear indication that this limitation can be overcome by manipulating the 4 parameters shown in the following figure. |
| **Illustration** |  <br>© Copyright Zhiliang Zhang |
| **Aims** | The project study will be a literature survey and develop an understanding of the scientific problem. The master study will *design and fabricate* ***super-dewetting surfaces,*** *which enable spontaneous transition from Wenzel to Cassie-Baxter state by manipulating surface chemistry, topology and gradients.*<br><br>**The topic has high breakthrough potential and great possibility for international journal publications.** |
| **Methods** | Mostly experimental and use the NTNU NanoLab |
| **References** | Contact us |

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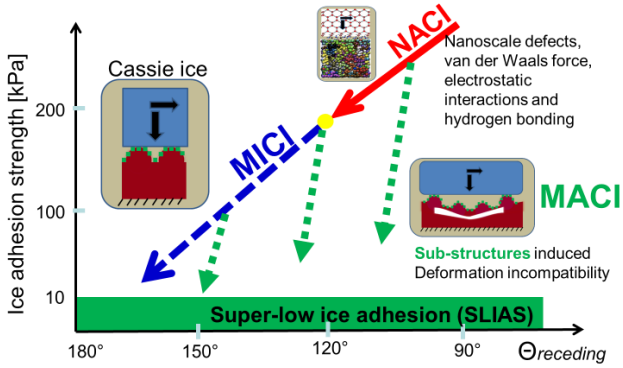
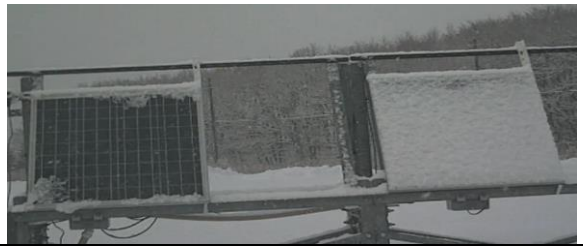
| **Title** | **Super-Low Ice Adhesion Surfaces** |
| **Supervising team** | Professor Zhiliang Zhang, zhiliang.zhang@ntnu.no<br>Professor Jianying He, jianying.he@ntnu.no<br>www.ntnu.no/nml |
| **Background** | Preventing icing on exposed surfaces is important for life and technology. While suppressing ice nucleation by surface structuring and local confinement is highly desirable and yet to be achieved, a realistic roadmap of icephobicity is to **live with ice, but with lowest possible ice adhesion**. **Super-low-ice-adhesion** (10 kPa) is defined as the adhesion where a cubic meter of ice can fall down by its own weight. Ice adhesion can be lowered by multiscale crack initiators, details see the reference. NTNU Nanomechanical Lab in the last years has created surfaces with ice adhesion as low as 5.7 kPa by introducing surface sub-structures. However, the surface sub-structures have not been optimized. The target is to reach the ice adhesion far below 1kPa. |
| **Illustration** | Unique concept<br>  <br>© Copyright Zhiliang Zhang<br>potential application<br>  |
| **Aims** | The project study will mainly focus on literature survey and get familiar with the established procedures to create super-low ice adhesion surfaces.<br><br>The master study will work on optimizing the surface sub-structures to reach the lowest possible ice adhesion, below 1kPa.<br><br>The topic has potential to patent the optimized sub-structures for lowest possible ice adhesion surfaces. |
| **Methods** | NTNU NanoLab will be used to synthesize the surface, lab at Department of Structural engineering will be used for ice adhesion testing. |
| **References** | http://pubs.rsc.org/en/content/articlelanding/2017/sm/c7sm01511a#!divAbstract |

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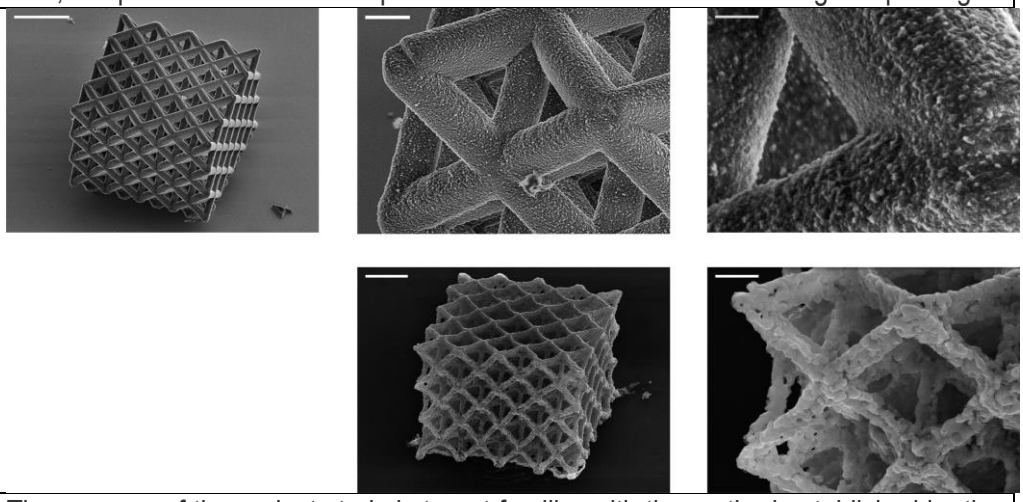
| **Title** | **3D Printing of Nano-Architected Metals** |
| **Supervising team** | Professor Zhiliang Zhang, zhiliang.zhang@ntnu.no<br>Professor Jianying He, jianying.he@ntnu.no<br>www.ntnu.no/nml |
| **Background** | In 3-D printing—also known as additive manufacturing—an object is built layer by layer, allowing for the creation of structures that would be impossible to manufacture by conventional subtractive methods such as etching or milling. Additive Manufacturing (AM) is a revolutionary technology with possibility of 3D printing any material, any shape, any quantity and in any fields, without the need for specialized tooling. Today's resolution of most commercially available metal AM processes is ~20–50 μm. However, thanks to a new technique developed at Caltech, for the first time, it is possible to create complex **nanoscale** metal structures using 3-D printing. |
| **Illustration** |  |
| **Aims** | The purpose of the project study is to get familiar with the method established by the Caltech group for Ni-based structures.<br><br>The aim of the master study is to explore the possibilities to extend the method to other metals, such as cu or aluminium. |
| **Methods** | Experimental study at the NTNU NanoLab |
| **References** | https://www.nature.com/articles/s41467-018-03071-9 |

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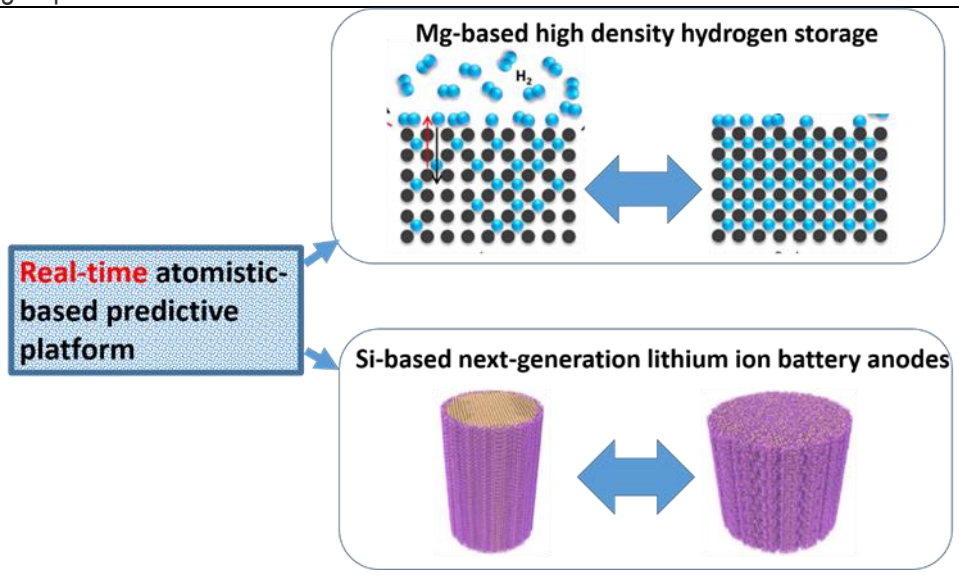
| **Title** | **Real-Time Molecular Dynamics Simulation for Nano-Engineering Energy Storage Materials** |
| **Supervising team** | Professor Zhiliang Zhang, zhiliang.zhang@ntnu.no<br>Professor Jianying He, jianying.he@ntnu.no<br>www.ntnu.no/nml |
| **Background** | The common characteristics of the energy storage materials can be generalized as charging / discharging / recharging processes. To atomistically simulate the rate-controlling charging/dis-charging/recharging processes in energy storage materials is very challenging since these processes are slow on the scale of seconds, minutes or even longer. This is an essential limitation for the classical molecular dynamics (MD) simulations which is based on solving Newton's equation of motion on the scale of thermal oscillations. The time increment for the classical MD simulations is about 0.5 to 2 femtoseconds ($10^{-15}$ second) and the longest time period today any MD can simulate is around 100 nanoseconds ($10^{-7}$ second). This limitation renders the classical MD inapplicable to slow kinetic processes. Recently a new method called diffusive molecular dynamics (DMD) which is able to atomistically simulate real time kinetic process (minutes or hours), has been developed by Prof. Michael Ortiz's group at Caltech. |
| **Illustration** |  <br>© Copyright Zhiliang Zhang |
| **Aims** | The project study will learn the classical molecular dynamics for simulating fast kinetics.<br><br>The master study will employ the DMD to evaluate the performance of nano-engineered energy storage materials. |
| **Methods** | Computational simulation using the LAMMPS code |
| **References** | Contact us. We will cooperate with Prof. Michael Ortiz at Caltech. |
| **Remarks** | If you are interested in programming and modeling, this is a good topic. |

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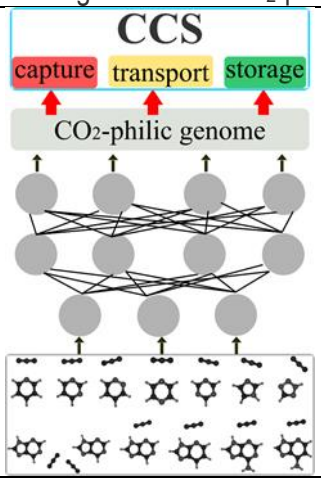
| **Title** | **Discover $CO_2$-phillic materials by Deep learning** |
| **Supervising team** | Professor Jianying He, jianying.he@ntnu.no<br>Professor Zhiliang Zhang, zhiliang.zhang@ntnu.no<br>www.ntnu.no/nml |
| **Background** | Designing $CO_2$-philic materials is a key to industry-practical Carbon Capture and Storage (CCS) technologies. Given the extremely large number of possible $CO_2$-philic chemical compounds, especially those organic functional groups, it is requisite to utilize the most powerful and accurate theoretical strategy to avoid the costly yet low-efficient trial-and-error first phase experimental material development. The current project aims to collect and create big data of accurate atomistic interactions and binding thermodynamics between $CO_2$ and a great variety of organic functional groups at varied temperature and pressure, and further to construct predictive models of $CO_2$-philicity using deep learning methods for identifying the universal $CO_2$-philic determinants and to design materials $CO_2$-philicity performances. |
| **Illustration** |  |
| **Aims** | The project study will focus on literature review and learn to use atomic simulations to generate the training data set.<br><br>The master study will learn to construct the predictive models by applying the deep learning method for $CO_2$-philicity. |
| **Methods** | Atomistic simulations by LAMMPS code |
| **References** | Contact us. |
| **Remarks** | If you are interested in programming and modeling, this is a good topic. |

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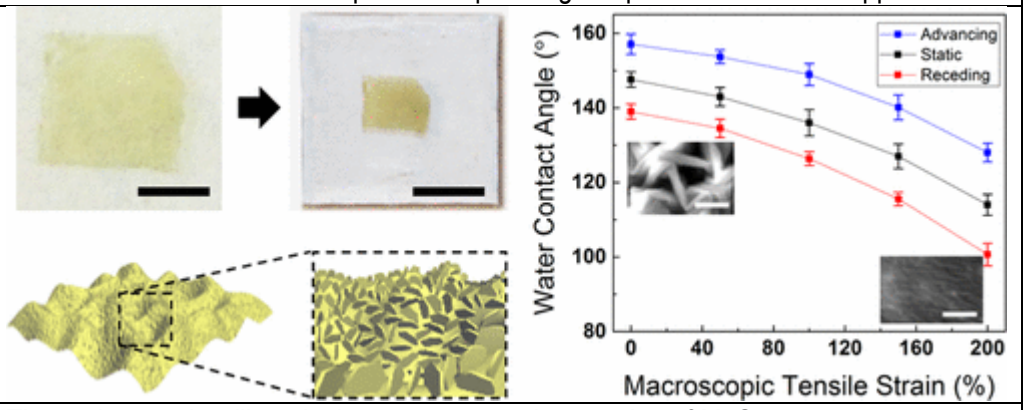
| **Title** | **Wetting on 2D single-layer molybdenum disulfide $MoS_2$** |
| **Supervising team** | Professor Zhiliang Zhang, zhiliang.zhang@ntnu.no<br>Professor Jianying He, jianying.he@ntnu.no<br>www.ntnu.no/nml |
| **Background** | Two dimensional (2D) transition metal dichchalcogenide crystals, consisting of a transition metal layer sandwiched between two chalcogenide layers in a trigonal prismatic structure, have attracted huge amounts of attention in recent years because of their distinctive electrical, optical and mechanical characteristics. Single-layer molybdenum disulfide ($MoS_2$), as the most representative 2D TMDCs, is a typical direct gap semiconductor with an intrinsic bandgap of about 1.8 eV due to quantum confinement. Also, single-layer $MoS_2$ shows excellent intrinsic electronic mobility and high on-off ratios. Such a host of fascinating properties of single-layer $MoS_2$ renders it great interesting both for fundamental studies of novel physical phenomena and for a wide range of applications in electronics systems, such as field-effect transistor, phototransistors, optoelectronics, nanoelectromechanical devices.<br><br>One of the interesting physical properties is surface wetting. The wettability of graphene has been substantially investigated, however, the wetting of $MoS_2$ structures has remained unexplored despite its great potentials in future applications. |
| **Illustration** |  |
| **Aims** | The project study will study the structures and properties of $MoS_2$.<br><br>The master study will study the interactions of the $MoS_2$ with water. |
| **Methods** | Both simulation and experimental work at NanoLab are possible, depending on the interest. |
| **References** | https://pubs.acs.org/doi/10.1021/acs.nanolett.6b05066<br>https://pubs.acs.org/doi/abs/10.1021/acs.nanolett.7b05433 |

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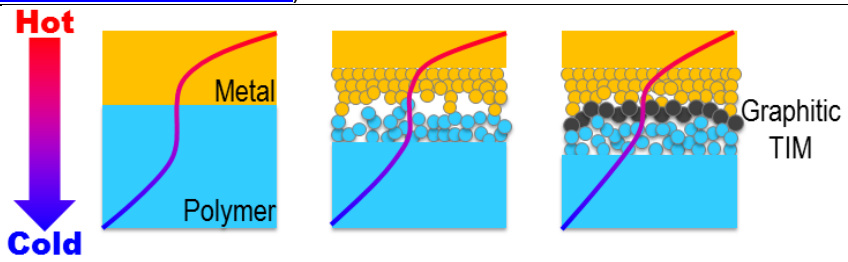
| **Title** | **Syntheses and Multiphysical Characterization of Ultra-thin Metal Film on Polymer Substrate** |
| **Supervising team** | Professor Jianying He, jianying.he@ntnu.no<br>Professor Zhiliang Zhang, zhiliang.zhang@ntnu.no<br>www.ntnu.no/nml |
| **Background** | Interfaces are everywhere in nature and engineering. Their properties are critical to a variety of processes and systems, ranging from thermal management of electronics, icing of solid surfaces to renewable energy applications. The intrinsic mechanisms that underlie interface properties are intertwined and inherently coupled with mechanical stresses. One extremely complex example, upon which this proposal is focused, is the heat conduction through metal and polymer interfaces with characteristic length scales ranged from a few nanometers to tens of micrometers. Due to the dissimilarity between metal and polymer, a major stress-coupled thermal resistance arises at the interface and impacts the functionality of the material system. Though the interface mechanical and thermal properties have been studied individually, the stress-coupled heat transfer is so far untouched either theoretically or experimentally.<br>Thermal interface materials (TIM) have been first introduced in polymer composites, and accepted in electronic systems as the route for improving the interface thermal conduction between semiconductor chips and metal heat spreaders, heat pipes and heat sinks. In the project, we will for the first time bring TIMs to the metal and polymer interface to optimize the stress-coupled thermal properties. Nanostructured graphitic TIMs, such as carbon nanotube (CNT), graphene and their derivatives, are expected to significantly improve the paths of heat transfer within the interface and smooth the dissimilarities of metal and polymer.<br>The project work is a part of FRINATEK Young Research Talent (YRT) project Engineering Metal-Polymer Interface for Enhanced Heat Transfer (HEFACE http://www.ntnu.edu/nml/heface). |
| **Illustration** |  |
| **Aims** | The project will synthesize nanoscale polymer-metal bilayer structure and characterize thermal-mechanical properties. |
| **Methods** | Both simulation and experimental work at NanoLab or NTNU Nanomechanical Lab are possible, depending on the interest. |
| **References** | http://www.ntnu.edu/nml/heface |