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# Laboratory study: Hydromechanical behavior of natural fractures

## Internship Description

Carbonate formations and reservoirs are often fractured. These fracture sets strongly influence the geo-plumbing of the reservoir. In other words, flow in the reservoir (both hydrocarbons and water), the ability to recover crude oil, production profiles from producing wells and the risk of bypassing oil are deeply affected by the fracture network. Because fracture aperture is stress sensitive natural fractures can hydraulically open or close as a result of reservoir pressure and stress changes associated to fluid injection or production.

We are looking for a highly motivated bachelor or master student who will be responsible for conducting a series of laboratory measurements. The purpose is to measure fluid flow as a function of pressure, normal load, and shear through a fracture within an artificial as well as real rock samples. This experimental work will include roughness measurements on fracture surfaces that are then correlated with individual experiment results.

Findings from this internship project will be integrated into the development of novel relationships and predictive capabilities between rock fractures and their hydraulic opening and closing behavior in response to reservoir pressure and effective stress changes.

We expect that this research will lead to publications, which the student can contribute to. Senior Research Scientist

## Deliverables/Expectations

We are seeking a B.Sc. (Bachelor of Science) or M.Sc. (Master of Sciences) student who is interested in the stated topic for his / her thesis research. The project is suitable for candidates who enjoy working in a laboratory and are interested in rock- and geo-mechanics, subsurface flow, or/and data analysis / statistics.

## Faculty Name

Carlos Santamarina

## Field of Study

Rock- and geo-mechanics or reservoir engineering



# Applications of reduced graphene oxide

## Internship Description

The project will make use of the method developed in the lab for the production of mesoporous reduced graphene oxide. Besides looking into the possibility to scale it up, the student will investigate possible applications for it namely in the environmental and energy-related fields.

## Deliverables/Expectations

Master the production of reduced graphene oxide;

Optimize the yield of the entire synthesis procedure and develop a strategy for scaled-up production;

Evaluate quantitatively the gas and energy storage capacity of the material.

## Faculty Name

Pedro Da Costa

## Field of Study

Chemistry / Materials Science / Physics



# Future Fuel for Advanced Combustion Engines

## Internship Description

Increasing focus on global warming and CO<sub>2</sub> emissions is pushing the engine technology to new frontiers. The overarching objective is to increase the efficiency of internal combustion engines so as to minimize the CO<sub>2</sub> emissions. Advanced engine technologies revolve around compression ignition concepts but diesel is not deemed to be suitable fuel for achieving higher efficiency and low pollutant levels. In this context, we are exploring new fuel formulations which can be produced at a lower cost from the refinery but can provide superior performance in the engine. The project will involve exploring the ignition and emission characteristics of such candidate future fuels.

## Deliverables/Expectations

Perform detailed physical/chemical characterization on select refinery stream fuels;  
Carry out ignition experiments in idealized reactor configurations of shock tube and rapid compression machine;  
Perform chemical kinetic modelling to develop surrogates for the fuels;  
Analyze the performance of new fuel in engine simulations;  
Recommend the optimal fuel formulation suitable for advanced compression ignition engines.

## Faculty Name

Aamir Farooq

## Field of Study

Mechanical Engineering, Chemical Engineering, Chemistry



# Modeling rock-fracture processes in geo-reservoirs and mining

## Internship Description

We are offering internship opportunities in the group Computational Earthquake Seismology (CES) at KAUST in the field of modeling rock-fracture processes in geo-reservoirs and mining environments. The goal is to understand, simulate, and “predict” the physics of earthquake ruptures (rock burst) that are induced by human (industrial) activities in geo-reservoirs that are characterized by a complex-geometry fracture network whose in-situ state is changed by external forcing (e.g. oil& gas extraction; fracking activities; external stimulation for instance of a geothermal reservoir; mining activities). Besides modeling the system response, we also want to extract a general understanding of earthquake nucleation, propagation and arrest within a semi-controllable system.

## Deliverables/Expectations

The deliverables include (1) a written report that could serve as an initial draft for a journal publication; (2) scientific poster that serves as a basis for a conference contribution; (3) documented work-flow and computer codes, including a short manual, to facilitate the continuation of the project by future students & researchers.

## Faculty Name

P Martin Mai

## Field of Study

Geology; Geophysics; Computer Science



## Big Data: Mess versus Value

### Internship Description

The problem of “messy” drilling and downhole data, and how to extract maximum value from it, is a pertinent challenge for the petroleum industry – in particular when it comes to advancing the understanding of near-wellbore physics and chemistry. This is particularly important since technological advancements, workflow optimizations and integrated project processes/execution are directly linked to a reduction in the cost of well construction, which generally is the largest expenditure item during field development.

We are looking for a highly motivated bachelor or master student who will be responsible for loading, processing, and analyzing continuous data streams from wellbores acquired with sensors during the drilling and reservoir monitoring process (e.g., measurement or logging while drilling). The purpose is to find in and extract from these data key information necessary to optimize drilling and improve our understanding of the processes ongoing in the near wellbore region.

Results from this internship project will be integrated into the development of automation systems that are capable of handling massive data streams from drill sites, maximize the quality of these data streams, find key information necessary to optimize drilling (i.e., lower cost), and help reduce risk, lost and non-productive time (i.e., prevent failures and accidents).

We expect that this research will lead to publications, which the student can contribute to.

### Deliverables/Expectations

We are seeking a B.Sc. (Bachelor of Science) or M.Sc. (Master of Sciences) student who is interested in the stated topic for his / her thesis research. The project is suitable for candidates interested in rock mechanics, geo-chemistry, or/and data analysis / statistics.

### Faculty Name

Tadeusz Patzek

### Field of Study

Drilling, production, or reservoir engineering.



# Expression, Purification, Characterization and Protein Catalysis of mutated Fluorescent Proteins

## Internship Description

A fluorescent protein variant was tailor-made as a suitable host for the incorporation of artificial metal centers through *in silico* removal of metal binding motifs and improvement of thermal, salt and solvent stability. Through introduction of mutations, metalloproteins are generated, which possess reactivities nature does not provide. These metalloproteins will be tested in aqueous catalysis reactions and the influence of mutations on selectivity and reactivity will be studied.

## Deliverables/Expectations

Students shall extend their general knowledge and skills in molecular biology and protein biochemistry. An emphasis will be put on expression, purification and characterization techniques. If capable mutant proteins will be crystallized to determine structural properties. Students will be taught to work independently on projects, yet strengthening their critical sense to develop new ideas. In the course of the internship students shall demonstrate this understanding during oral presentations and one final written report.

## Faculty Name

Magnus Rueping

## Field of Study

Chemistry/Biochemistry/Molecular Biology





# Earthquake source modeling with complex fault geometry

## Internship Description

We are offering internship opportunities in the group Computational Earthquake Seismology (CES) at KAUST in the field of earthquake source modeling for understanding (a) the physics of earthquake ruptures; (b) the radiated seismic ground motions and their effects on seismic hazard estimation. The focus in these projects is on the inclusion of the geometrically complex fault system on which in particular large earthquakes happen. Case studies of particular interest are transtensional strike-slip fault systems with segmented step-over faults (e.g. the fault system in the Gulf of Aqaba, Husavik Flatte Fault (Iceland); faults in Southern California), and complex-geometry subduction faults (e.g. South America; Sumatra; Makran region) and the generation of possible tsunamigenic events.

## Deliverables/Expectations

The deliverables include

- (1) a written report that could serve as an initial draft for a journal publication;
- (2) scientific poster which serves as a basis for a conference contribution;
- (3) documented work-flow and computer codes, including a short manual, to facilitate the continuation of the project by future students & researchers.

## Faculty Name

P Martin Mai

## Field of Study

Geology; Geophysics; Computer Science



# Optical and Electrical Characterization of Thin Films for Photovoltaic Applications

## Internship Description

The student(s) will perform different steady-state and time-resolved optical and electro-optical experiments on thin films and photovoltaic devices that use organic and hybrid materials as photoactive layer for solar energy conversion. Depending on the students' interest, skills, previous experience, and progress throughout the project, these experiments can range from steady-state spectroscopy (UV-Vis absorption, ellipsometry), sensitive absorption measurements (photo-thermal deflection spectroscopy (PDS)), photo-induced absorption spectroscopy (PIA), and charge carrier mobility measurements (SCLC, CELIV, TOF) using home-built experimental setups to ultrafast photoluminescence spectroscopy experiments that use state-of-the-art femtosecond laser systems in combination with Streak Camera detectors.

## Deliverables/Expectations

Interest in optics, (ultrafast) lasers, optical spectroscopy, specifically time-resolved optical spectroscopy, and electrical measurements; experience with programming (LabView, Matlab) languages and data analysis software (Origin or equivalent) beneficial, but not a strict requirement.

## Faculty Name

Frederic Laquai

## Field of Study

Physics, Physical Chemistry, Material Science



# High Pressure Heterogeneous Autoignition of Hydrocarbon and Syngas Fuels

## Internship Description

Work with postdoc on new high pressure vessel to measure the autoignition characteristics of gaseous fuels

## Faculty Name

William Roberts

## Field of Study

Mechanical Engineering, Chemical Engineering, Aerospace Engineering, Physics.



# Engineering Chemical Reactions with Machine Learning

## Internship Description

Improving combustion engines and industrial chemical reactors requires a detailed understanding of complex chemical reaction networks. The project aims to radically increase the pace of innovation by developing machine learning tools to engineer chemical reactions. The student will work with “big data” sets comprising various reaction properties. These large data sets will include experimental values augmented with simulated values generated with multi-scale models. Artificial neural networks and genetic algorithms will then be trained to predict a wide range of combustion properties using a limited number of input parameters. The machine learning predictions will be compared against detailed multi-scale models to develop novel cloud-based tools for understanding combustion in complex systems. The candidate will develop new software incorporating new uncertainty-analysis features, experimental templates, open-access formats, and open-source software for data mining and predictive simulations. The candidate will receive scientific guidance in developing the various aspects of the cyber-infrastructure, but must have the appropriate skills, technical expertise, and prior experience to be successful. Excellent chemical engineering and computer programming skills are required.

<https://cloudflame.kaust.edu.sa>

## Deliverables/Expectations

The student is expected to participate in writing journal publications and presenting research at conferences: Weekly updates on research progress

Presentation of your research at least three times during course of internship

Remaining in the lab/office during regular business hours (9am to 5pm)

Written final report on internship projects.

## Faculty Name

Mani Sarathy

## Field of Study

Computer Science, Computer Engineering, Software Engineering, Chemical Engineering



## Spin-orbitronics in Anderson regime

### Internship Description

This topic concerns the exploration of spin-charge conversion processes (such as spin Hall effect and spin galvanic effect) in strongly disordered materials using quantum transport calculations. In particular, we are interested in understanding how these processes behave in through Anderson transition, when the material transforms from a metal into an insulator.

### Deliverables/Expectations

Produce solid numerical results of the conductance and spin density as a function of disorder strength in two dimensional electron gases using the KWANT code.

Determine the scaling laws that govern spin-charge conversion processes at Anderson transition

### Faculty Name

Aurelien Manchon

### Field of Study

Condensed Matter Physics, Magnetism



# Time resolving imaging of fundamental photo-physical processes of photoactive materials

## Internship Description

We propose to use four-dimensional scanning ultrafast electron microscopy (4D S-UEM) to take time-resolved images (snapshots) at the nanometer and femtosecond scales to provide real-space information on the fundamental photo-physical processes including exciton and carrier generation, separation, trapping, and recombination for several photoactive materials surfaces which are relevant to emerging photovoltaics technologies.

## Faculty Name

Omar F. Abdelsaboer

## Field of Study

Physical Chemistry



# Optical and electronic properties of Inorganic-organic (perovskite) bulk hybrid system for optoelectronic applications

## Internship Description

The overall aim of the project is to study optical and electronic properties of the inorganic-organic bulk hybrid system. Organo-halide perovskite (e.g.  $\text{CH}_3\text{NH}_3\text{PbI}_3$ ) will be used as organic counterpart. Solution-processed organo-halide perovskite (OHPVK) exhibits long electronic carrier diffusion lengths, high optical absorption coefficients and impressive photovoltaic device performance. The real potential of OHPVK is yet to be used for other optoelectronic applications such as waveguide, light emitting diode etc. In order to do that we need to highlight the fundamental questions that needed to be addressed regarding the carrier-recombination and charge transport properties. Both of these aspects will be studied in depth by using different characterization techniques as mentioned below. We will introduce metal-oxide based nanostructures as an inorganic counterpart. Metal-oxides are an interesting range of materials and we will exploit the unique properties of metal-oxide based nanostructures in order to modify the properties of the organic/metal-oxide hybrid system.

Students will be involved partly in preparation and synthesis of the materials. For characterization students will be trained to use photoluminescence (PL) and time-resolved spectroscopy (TRS), IV and absorption (UV-Vis) techniques. Students will have hands-on experience on the aforementioned techniques and will be able to gain research experience on the field of organic-inorganic hybrid systems. At the end of the laboratory work, students will be directed to write their findings in terms of report.

The time frame of the project needs at least 4-6 months.

## Faculty Name

Iman Roqan

## Field of Study

Semiconductor spectroscopy



# First-principles investigation of superlattices of 2D materials

## Internship Description

The aim of the project is to develop basic insight into the properties of superlattices consisting of 2D materials by first-principles calculations (density functional theory; Boltzmann transport; non-equilibrium Green's function approach). In general, superlattices are of interest in the field of thermoelectrics, because they give access to designing the phonon scattering and therefore to influencing the thermal transport. Stacking of 2D materials in addition modifies the electronic states at the Fermi level and thus has the potential to enhance the figure of merit. The question of ion absorption in superlattices is of key importance for battery applications. Because of their high surface-to-volume ratio, 2D materials are intensively studied for various kinds of sensors, while superlattices so far have been considered only rarely in this context.

## Faculty Name

Udo Schwingenschlogl

## Field of Study

Computational Materials Science





# Dynamics of MEMS for mechanical computing

## Internship Description

The dynamic behavior of micro-electromechanical systems MEMS devices will be simulated to achieve logic functions such as OR, AND gates. The project will require building a model for MEMS resonator and running computer simulations to help in the design of these resonators; so that they are eventually fabricated and tested. The project requires basic programming skills, which are commonly mastered at the undergrad level of engineering.

## Faculty Name

Mohammad Younis

## Field of Study

Mechanical engineering



# Simulations of Large Scale Turbulent Flames using OpenFOAM

## Internship Description

Develop computational fluid dynamics (CFD) simulation code based on OpenFOAM, open-source CFD code modules, to describe large scale turbulent flames relevant to natural fire or industrial combustors.

## Faculty Name

Hong G. Im

## Field of Study

Mechanical/Aerospace/Chemical Engineering, Applied Physics/Mathematics



# Simulations of Spray and Combustion in Engines

## Internship Description

Develop computational fluid dynamics (CFD) simulation code based on OpenFOAM, open-source CFD code modules, to describe liquid spray injection, atomization, droplet interactions and combustion; and will conduct preliminary simulations for demonstration.

## Faculty Name

Hong G. Im

## Field of Study

Mechanical/Aerospace/Chemical Engineering, Applied Physics/Mathematics



# New Materials and Process for High Performance Organic Solar Cells

## Internship Description

Successful commercialisation of organic solar cells requires a combination of high performance, stability, and low cost processing. We have an active research program to address each of these requirements. High efficiency materials design requires optimal light absorption across the solar spectrum, effective charge separation and photocurrent generation. Our synthetic strategies are focussed on new electron donor and acceptor combinations which can accomplish this process efficiently, and one of our projects involves organic synthesis of new conjugated aromatic semiconducting materials. The second project involves the characterisation of these materials using optical and electrical methods, as well as fabricating solar cell devices. Our development of a new isoindigo polymer has demonstrated a record power conversion efficiency of over 9% in a device without a thermal treatment processing step and without the use of additives in the formulation. Reductions in processing energy and time are essential for this technology to be competitive as an energy source, therefore eliminating thermal treatment is an important achievement.

## Faculty Name

Iain McCulloch

## Field of Study

Chemistry



# Novel highly efficient hole transporting layers for perovskite solar cells

## Internship Description

This project is focusing on an emerging and highly promising technology, perovskite solar cells. Novel hole transporting materials synthesized in our group will be utilized. The successful candidate will gain experience on device fabrication, electrical and morphological characterization of the perovskite solar cells.

## Faculty Name

Iain McCulloch

## Field of Study

Material Science and Engineering, Applied Physics, Chemistry



# Development of Water-Soluble Semiconducting Polymers for Organic Bioelectronic Devices

## Internship Description

Current bioelectronic materials used to transduce signals across the biotic/abiotic interface, are mainly either semiconducting silicon or conducting metal contacts, while recent progress in research into organic bioelectronics is limited by standard commercially available materials that are not explicitly designed for bio applications. Specifically, two emerging areas of research interest are ionic conductivity modulation and facile conducting polymer bio-functionalization. Organic semiconducting devices employed in organic bioelectronics are potentially advantageous as they have no insulating oxide barrier between the material and biological interface. Due to their ‘soft’ nature and size compatibility, ions are free to penetrate into the bulk of the active material, leading to an exponential increase in signal to noise ratio. Incorporating a source and drain at either side of the semiconductor channel, and gating performed by the electrolyte, creates an organic electrochemical transistor (OECT). Our objective is to design a platform of water-soluble, semiconducting polymer devices specifically for application in the range of emerging bio-organic electronic applications. One project will involve the synthetic design of dopable conducting, ion transport polymers, with inherent aqueous solubility with appropriate reactive groups for bio compatibility and grafting, or alternatively smart chelating groups which can either induce an optical signal on capture of a target species, or can be electrically modulated to release the species. Such species include ions and neurotransmitters. A second project will involve the physical characterisation of new bioorganic polymer materials, as well as fabrication, optimisation and testing of simple devices which utilise these exciting new materials.

## Faculty Name

Iain McCulloch

## Field of Study

Biophysics, Physics, Chemistry, Material Science



# Laser Deposited Nanostructures for on-Chip Energy Storage

## Internship Description

This project will involve fabrication of microsupercapacitors using pulsed laser deposition of nanostructured electrodes and direct-write patterning for energy storage applications. In this project, the student will be trained to use pulsed laser deposition to deposit nanostructured cathode materials for microsupercapacitors, which are useful for onchip energy storage. The student will make nanostructured films of transition metal oxides or chalcogenides and study their properties. These films will be characterized to insure the formation of the appropriate crystalline phase and desired nanoscale morphology. The student will then pattern the deposit films using direct-write methods or lithographic techniques. Different solid state electrolytes will be used to fabricate the microcapacitor devices. The effect of material nanostructure, feature size, and device design on the speed, power, and energy density of the resulting devices will be studied. Electrochemical and spectroscopic measurements will be done by the student during device cycling (in-situ) and afterwards to understand electrode behavior during the electrochemical reactions, and to optimize electrode performance.

## Faculty Name

Husam Alshareef

## Field of Study

Double Major Chemistry (3.95) and Physics (4.0)



## Optical properties of InGaN/ GaN and AlGaN/GaN multi- quantum well grown on Ga<sub>2</sub>O<sub>3</sub>

### Internship Description

III- nitride semiconductors are the most suitable source for blue and deep UV LEDs and LD lasers for different potential applications such as water sterilization, skin treatment and security. Therefore, the optical efficiency should be optimized for such applications. Two dimension multiple quantum well (MQW) carrier confinement are necessary to increase the efficiency. We investigate the optical properties of III- nitrides quantum well grown on new class of substrate by mean of photoluminescence (PL) and time- resolved spectroscopy (TRS). The student project will be investigation of the optical properties of the specific structure of AlGaN/GaN MQW and we compare the results with that grown on common used substrates using photoluminescence (PL) techniques including PL selectively excitation and PL temperature dependence. TRS measurements will be carried out using ultrafast laser and streak camera ( detecting system). TRS measurements will study the carrier confinement mechanism and the carrier life time by exciting the material above and below quantum barrier energy. The second part of the project will be designing new devices using special software to optimize the structure and predict the performance which assists in growing the samples/ devices. This project needs 3-5 months to be completed.

### Faculty Name

Iman Roqan

### Field of Study

Semiconductor spectroscopy





# Chemical Kinetics of Novel Biofuels

## Internship Description

Biofuels are becoming increasingly important in the world's energy infrastructure and their use has steadily been increasing in Europe and the U.S. With a number of candidate biofuels, a concentrated effort must be spent on choosing the optimal fuel that can be produced in a cost-effective manner and deliver the best performance within the engine. The student will initially work on choosing a few candidate biofuel molecules for investigating experimentally in the laboratory. Thereafter, he/she will perform a series of experimental studies on the selected fuels to understand their chemical kinetics behavior.

## Deliverables/Expectations

- Perform life-cycle-analysis to select candidate biofuels
- Characterize various biofuel molecules in terms of their physical properties
- Conduct detailed experiments on the chemical kinetics behavior of these biofuels using shock tube and rapid compression machine
- Run validated chemical kinetics models to estimate the performance of studied biofuels in an engine
- Show how the new fuel leads to improvement in engine efficiency and reduction in emissions

## Faculty Name

Aamir Farooq

## Field of Study

Mechanical Engineering or Chemical Engineering



# Enhancing Weather Downscaling and Forecasting

## Internship Description

Global weather products can only be computed at coarse resolution, and therefore cannot resolve important sub-grid scale features such as clouds and topography. Downscaling methods are used to compute local weather forecasts at high resolution from the global products. Nudging and Spectral Nudging methods are popular techniques for constraining local models with global products. The goal of the internship is to explore and test more advanced downscaling techniques based on the recently developed continuous data assimilation framework and/or the ensemble Kalman filter.

## Faculty Name

Ibrahim Hoteit

## Field of Study

Applied Mathematics, Meteorology, or any related field



# Thin Film Alloys for Na-ion Battery Applications

## Internship Description

The student will deposit thin film alloys based on Na and group 14 elements (eg Sn or Sb) and evaluate the effect of their structure and morphology on Na-ion battery performance. The student will also perform in-situ material analysis (Raman, FTIR, XRD) to understand the chemical changes taking place during battery cycling.

## Faculty Name

Husam Alshareef

## Field of Study

Chemistry, Physics, or Materials Science



## Transparent hybrid organic-inorganic perovskite solar cells

### Internship Description

Fabricate and test solution-processed semi-transparent perovskite solar cells. Characterize transmission and optimize fabrication steps and layers to achieve optimal performance. Potential applications range from wearable power generation to building and automotive integration and hybrid tandem solar cells.

### Faculty Name

Aram Amassian

### Field of Study

Solar energy, materials science and engineering



## Optical properties of AlGaN AlInN multi-layer nanorods.

### Internship Description

AlGaN materials are the most suitable source for deep UV LEDs and LD lasers for different potential applications such as water sterilization, skin treatment and security. Therefore, the optical efficiency should be optimized for such applications. Two dimension (quantum well) and three dimension (nanorods) carrier confinement are necessary to increase the efficiency. We study the optical properties of AlGaN quantum well and nanorods by means of photoluminescence (PL) and time-resolved spectroscopy (TRS). The student project will be investigation of the optical properties of specific structure of AlGaN/AlInN nanorods (each nanorod contains multi layers of AlGaN and AlInN to give additional confinements) and we compare the results with AlGaN/AlInN quantum well using PL techniques including PL selectively excitation and PL temperature dependence. The second part of the project is TRS measurements using ultrafast laser attached to second harmonic generator (excitation source) and streak camera (detecting system). TRS measurements study the carrier confinement mechanism. This project needs 3 to 5 months to be completed.

### Faculty Name

Iman Roqan

### Field of Study

Semiconductor spectroscopy



# Synthesis of Novel Pincer complexes

## Internship Description

The student will work on the design and synthesis of 2-amino-pyridine based pincer ligands (3-10 steps) and the preparation of their corresponding transition metal complexes. Students will be trained on standard organic synthesis knowledge and Schlenk skills.

## Faculty Name

Kuo-Wei Huang

## Field of Study

Chemistry



# Novel Phenomena at perovskite interfaces and superlattices

## Internship Description

Superlattices of perovskite oxides often have properties distinguished from their bulk phases. Investigation of these properties is at the forefront of modern condensed matter physics and materials science. In particular, after the observation of a highly mobile two-dimensional electron gas at the interface between  $\text{LaAlO}_3$  and  $\text{SrTiO}_3$ , engineered interfaces are emerging as new horizon for various applications. Using the density functional theory, the project aims at determining the magnetic, electronic, and optical properties of possible perovskite interfaces and superlattices.

## Deliverables/Expectations

Report. Seminar presentation

## Faculty Name

Udo Schwingenschlogl

## Field of Study

Physics, Materials Science, Chemistry, Electrical Engineering



# Role of non-classical hydrogen bonding in organocatalysis

## Internship Description

The student will utilize kinetic (NMR, IR, etc) and computational tools (DFT calculations) to elucidate the role of hydrogen bonding network and in particular the non-classical hydrogen bonding in the thiourea and guanidine-based organocatalysis.

## Deliverables/Expectations

Assist in the kinetic study and DFT calculations.

## Faculty Name

Kuo-Wei Huang

## Field of Study

Chemistry





# First principles modeling of hybrid organic-inorganic perovskites

## Internship Description

Hybrid organic-inorganic perovskite solar cells have recently emerged as the next-generation photovoltaic technology. Most of the work has been focused on the prototype MAPbI<sub>3</sub> perovskite (MA= Methylammonium = CH<sub>3</sub>NH<sub>3</sub><sup>+</sup>) and its analogues that have lead to power conversion efficiencies in excess of 15%. Despite the huge success, these materials are still non-optimal in terms of optical absorption as the bandgaps are ~1.6 eV and greater. Thus, investigation and development of perovskites with bandgaps closer to optimal, allowing enhanced spectral absorption, is of great interest. The aim of this project is to perform first-principles calculations to study the structural, optical, and electronic properties of new derivatives of MAPbI<sub>3</sub> in which the organic MA cation is replaced by other organic amines of similar size and/or the Pb cation is replaced by similar elements.

## Faculty Name

Udo Schwingenschlogl

## Field of Study

Physics, Materials Science, Chemistry, Electrical Engineering



# Catalysis for energy conversion

## Internship Description

The following topics can be selected based on student's interest:

- \* Photocatalysis for hydrogen generation
- \* Advanced electrocatalysis for water splitting
- \* Electrochemical CO<sub>2</sub> reduction

Projects will involve: material synthesis, electrochemical measurement, photocatalytic measurement, and various characterizations (SEM, UV-VIS, IR, XRD, XPS, gas / liquid / ion chromatography).

## Deliverables/Expectations

The internship student will gain fundamental knowledge on energy conversion and concept of potentials.

The student is expected to work full-time.

The results are utilized for publications.

## Faculty Name

Kazuhiro Takanabe

## Field of Study

Physical Chemistry / Catalysis



# Adhesion phenomena across interfaces with spatially heterogeneous adhesive properties

## Internship Description

The project aims to explore the effect of heterogeneities on the mechanical behavior of bonded interfaces through integrated experiments and simulations. The research seeks to systematically design multiple sites of potential crack pinning across the interface, able to trigger sequential events of initiation, propagation and crack arrest, thus promoting macroscopic variations of strength and toughness. Inspiration in the search for such novel material configurations is derived from those observed in nature. Successful design of these bio-inspired interfaces can lead to quite interesting technological applications.

## Faculty Name

Gilles Lubineau

## Field of Study

Mechanical engineering, Material science, civil engineering



# Ultra Sensitive Sensors based on Nanotubes Porous Networks

## Internship Description

This project will focus on design, development and implementation of a family of ultra sensitive sensors taking advantage of tunnelling effects in carbon nanotube porous networks. The intertube junctions will be customized by using different materials depending of the sensing needs (moisture, special gas, deformations..) The student will be in charge of defining a simple phenomenological model for each sensing mechanism, of choosing the best material and microstructure configuration for each sensing need and to manufacture, test and validate the resulting prototype. This study is relevant for applications in structural health monitoring and for continuous tracking of biological systems. The student is expected to participate in writing journal publications and presenting research at conferences.

## Deliverables/Expectations

### Faculty Name

Gilles Lubineau

### Field of Study

Mechanical Engineering



# Mechanical Integrity of Bio-Inspired Composites

## Internship Description

The candidate will have to explore highly innovative ideas in the field of bio-inspired interfaces and materials. The focus will be on the design of new patterned interfaces, processed by laser treatment, with improved toughness and delamination resistance. The candidate will have to go through an extensive literature review, both on fracture engineering but also on available biological systems. Then, he will participate in defining the strategy for the patterning and be in charge of the exploration/test and validation of the concept. The student is expected to participate in writing journal publications and presenting research at conferences.

## Deliverables/Expectations

### Faculty Name

Gilles Lubineau

### Field of Study

Mechanical Engineering



## Mechanical properties of new integrated flexible electronics based on doped thermoplastics

### Internship Description

An internship opportunity is available within the framework of a research project related to future flexible electronics. These are usually made of a transparent electrode (ITO) deposited on a polymer substrate. Such design results in loss of integrity when cracks develop in the thin brittle electrode. This project intends to characterize mechanical properties of new technologies for which the electrode and the substrate are merged together into a single active layer. The project will cover fatigue dependent properties as well as piezoresistive effects. The student is expected to participate in writing journal publications and presenting research at conferences.

### Faculty Name

Gilles Lubineau

### Field of Study

Mechanical Engineering



# Mechanical integrity of thermoplastics structural composites

## Internship Description

A studentship opportunity is available in close collaboration with a major industry for the optimization of thermoplastic tapes for automotive applications. A micromechanical tool has been developed in the team for the simulation of integrity knowing the microstructure of the composite. The objective will be to use and improve that tool in order to determine the main parameters influencing on the final performance of the tape. The involved student will become expert in Abaqus as well as in composite characterization. The involved student is expected to participate in writing journal publications and presenting research at conferences.

## Faculty Name

Gilles Lubineau

## Field of Study

Mechanical Engineering



# Experiments on High-Speed Multi-Phase Flow

## Internship Description

The project will use high-speed video cameras to study the motions of drops and bubbles inside high-speed water-flow through a small channel. Two high-speed cameras will be used to follow the trajectories of the droplets and small bubbles and record their breakup. The aim of the work is to see how the smallest droplets or bubbles are generated by the turbulent flow-field. This study is relevant for applications in the petrochemical industry.

## Deliverables/Expectations

Perform experiments in the *High-Speed Fluids Imaging Laboratory* under the supervision of Sigurdur Thoroddsen. Write a final report describing all the experiments performed and reducing the data. Write a description of experimental techniques for others to continue the work.

## Faculty Name

Sigurdur Throddsen

## Field of Study

Fluid Mechanics, Mechanical Engineering or Chemical Engineering





# Monitoring subsidence due to groundwater pumping in central Arabia

## Internship Description

Excessive pumping and use of groundwater aquifers in the Middle East is a serious problem, leading to aquifer depletion, permanent compaction and shortage of usable water. One effective way of monitoring the aquifer usage is satellite radar mapping of cm-level subsidence due to groundwater pressure decrease in the aquifer systems. In this project, we plan to use such satellite radar observations of areas in central Arabia to map out the extent and magnitude of ongoing subsidence. The results will provide an overview of the problem of groundwater overuse and may help the authorities to take the necessary actions.

## Deliverables/Expectations

The student(s) will learn how to process satellite radar data using Linux/shell based program routines. They will also need to learn how to work with the outcome (e.g. in Matlab), display the results, and to provide quantitative assessment of the level of subsidence and extent of the groundwater over use problem. The results should be summarized in a short report at the end of the internship.

## Faculty Name

Sigurjon Jonsson

## Field of Study

Earth Science, Environmental science and engineering



# Constraining Earth Fluid Motion Models with Satellite Images

## Internship Description

Developing exact mathematical models to stimulate and predict oceanic and atmospheric motions is a difficult process because of the complex multi-physical interactions. Satellite images provide a powerful tool to extract in detail some information at various scales that could be used to reduce the uncertainties in the numerical models. Constraining the models with those images requires introducing some physical knowledge about the studied motion. The goal of this project is to study approaches that would allow to directly constraining and calibrating numerical models with structures extracted from images.

## Deliverables/Expectations

Literature review of images assimilation methods. Explore and study the efficiency of ensemble Kalman filtering methods for images assimilation. Implement and assess performance with numerical test models (e.g. Shallow water)

## Faculty Name

Ibrahim Hoteit, Ganesh Sundaramoorthi

## Field of Study

Applied Mathematics, Earth Sciences and Engineering, Electric Engineering or any related field.



# Wafer-scale patterned growth of vertically aligned carbon nanotubes

## Internship Description

The project aims to optimize the patterned growth of vertically-aligned carbon nanotubes (VA-CNT) on wafers sized up to 4-inches using a plasma-enhanced chemical vapour deposition reactor. The first part will be to optimize the large-area and/or patterned deposition of the metal catalyst. Afterwards, different recipes for the growth of VA-CNT will be explored and, ultimately, a collection of wafers containing from SWCNTs to MWCNTs should be obtained. Characterization of the VA-CNT will be carried out using a collection of tools such as electron microscopy and Raman spectroscopy.

## Deliverables/Expectations

Si wafers coated with a thin layer of a transition metal active for CNT growth  
Si wafers coated with a patterned thin layer of a transition metal active for CNT growth  
Mats of VA-CNTs grown on 4"-wafers  
Patterned mats of VA-CNTs grown on 4"-wafers  
One poster or oral communication at a conference  
Final written report

## Faculty Name

Pedro Da Costa

## Field of Study

Materials Science and Engineering / Chemistry / Physics



# Direct Numerical Simulation of Turbulent Combustion at High Pressures

## Internship Description

Learn the in-house direct numerical simulation code and modify for high pressure and high Reynolds number reacting flow problems. Pilot simulations of canonical combustor configurations will be conducted as a demonstration of the new capabilities.

## Deliverables/Expectations

Modified DNS code with specific problem configurations. Pilot simulations and analysis for demonstration.

## Faculty Name

Hong G. Im

## Field of Study

Mechanical/Aerospace/Chemical Engineering, Applied Physics/Mathematics



## Fuel Design

### Internship Description

Students will develop state of the art tools to determine the technical and environmental performance future fuels. He/she will also be involved in experiments in engines, flow reactors, and flames to improve models and to develop a deeper understanding of future fuel combustion performance. The student should have interest and/or expertise in one of the following areas: computer programming, life cycle assessment, reaction engineering, chemical thermodynamics, quantum chemistry, and combustion simulations. The student will use their knowledge to better understand fuel formation and combustion in engines. The student is expected to participate in writing journal publications and presenting research at conferences. <http://cpc.kaust.edu.sa>

### Deliverables/Expectations

Weekly updates on research progress

Presentation of your research at least three times during course of internship

Remaining in the lab/office during regular business hours (9am to 5 pm)

Written final report on internship projects.

### Faculty Name

Mani Sarathy

### Field of Study

Chemical Engineering, Mechanical Engineering, Chemistry



# Quantifying and reducing uncertainties in earth fluid models

## Internship Description

Earth fluid models are subject to different sources of uncertainties. We will work on developing and implementing Bayesian inference approaches to quantify and reduce uncertainties in these models with focus on applications related to the coastal ocean, e.g. storm surges, tsunamis, oil spill, waves, etc. We envision using statistical and polynomial chaos-based techniques to build surrogate models that can be used to reduce the computational burden of the sampling step in the Bayesian inference.

## Faculty Name

Ibrahim Hoteit, Omar Knio

## Field of Study

Applied Mathematics, Earth Sciences and Engineering, or any related field



# Biomedical Sensor Development

## Internship Description

The project involves design, development and implementation of a laser-based biomedical sensor. The sensor will be used to monitor human breath for disease diagnostics. The student will work on studying the electromagnetic spectrum of various substances, choosing the candidate optical transitions, setting up the laser-based optical setup and performing laboratory measurements to detect species concentration in trace quantities. The student will gain expertise in spectroscopy, statistical thermodynamics, optical engineering and mechanical engineering.

## Deliverables/Expectations

- Spectral line selection using state-of-the-art spectroscopic models
- Set up optical setup for performing validation measurements
- Demonstration of the sensor in "simulated breath" mixtures
- Application of the sensor to breath samples of patients

## Faculty Name

Aamir Farooq

## Field of Study

Mechanical Engineering or Chemical Engineering