KAUST VISITING STUDENT RESEARCH PROGRAM PROJECTS FOR PHYSICAL SCIENCE AND ENGINEERING

The Visiting Student Research Intern Program is an opportunity for exceptionally qualified international baccalaureate and Masters students to conduct research with faculty mentors in basic and applied research projects. The duration of the internship program can range between four to six months depending on the project.

In the Physical Science and Engineering Division (PSE) our mission is to create knowledge pertaining to matter at all scales - nano, meso and macro - and in all forms, from bulk, to divided colloids and fluids: as well as to create knowledge about the interaction of matter with external stimuli in order to design new materials and technologies that can address our quest to mitigate or even solve some of the major challenges that we face in the world today.

Our graduate students and internationally renowned Faculty focus on challenges related to energy and the environment. We also focus on exploration and manipulation at the nanoscale.

The division has four faculties: Chemistry and Chemical Engineering, Earth Science and Engineering, Material Science and Engineering, and Mechanical Engineering.

Who is Eligible?

3rd Year Baccalaureate or Masters Students

GPA 3.5/4.00 (14/20 ECTS B)

Strong verbal and written English Skills

Application Requirements

Official Transcript(s) in English from current and previous institutions

Letter of recommendation from faculty member in field of student

Valid Passport

Benefits

$1000USD Monthly Stipend
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Visa and Airfare Fees
Health Insurance
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applications accepted year-around

Data Assimilation into large dimensional systems

Faculty Mentor
Professor Ibrahim Hoteit, Earth Science and Engineering

Internship Description
Develop and test efficient data assimilation (such as ensemble Kalman and particle filters and smoothers, 4DVAR, etc) schemes for state and parameters estimation of large dimensional systems. Numerical experiments will be conducted with simplified atmospheric, oceanic, or hydrological models.

Deliverables/Expectations

Report and presentation

Field of Study: Physical Oceanography or any related field

Duration of Internship: 3 months

Ocean Modelling and remote sensing the Red Sea circulation and ecosystem

Faculty Mentor
Professor Ibrahim Hoteit, Earth Science and Engineering

Internship Description
Study Red Sea circulation and ecosystem using high resolution ocean models simulation, (e.g. MIT ocean general circulation model - MITgcm and European Regional Seas Ecosystem Models - ERSEM), and state-of-the-art remote sensing techniques with available in-situ observations.

Deliverables/Expectations

Report and presentation

Field of Study: Physical Oceanography or any related field

Duration of Internship: 3 months

Laser-based Sensor Design and Development

Faculty Mentor
Professor Aamir Farooq, Mechanical Engineering

Internship Description

The project involves design, development, and implementation of a laser-based optical sensor. The sensor will be used to monitor environmental pollutants (e.g., NOx, CO) or greenhouse gas emissions (e.g., N2O, CH4, CO2). The student will work on studying the electromagnetic spectrum of various molecules, choosing the candidate optical transitions, setting up the laser-based optical setup, and performing laboratory measurements to detect species concentration in trace quantities. Advanced sensing strategies, such as wavelength modulation, cavity-enhancement and frequency combs will be utilized. The student will gain expertise in spectroscopy, statistical thermodynamics, machine learning, optical engineering, and mechanical design.

Deliverables/Expectations

- Spectral line selection using state-of-the-art spectroscopic models
- Design of optical, electronic and mechanical components of the sensor
- Laboratory validations of the sensor performance
- Field testing for trace gas detection

Field of Study: Physics, Electrical Engineering, Mechanical Engineering, Chemical Engineering

Duration of Internship: 3 months

Rupture Dynamics on Rough and Segmented Faults

Faculty Mentor
Professor P Martin Mai, Earth Science and Engineering

Internship Description
In this project, the student will conduct numerical experiments to study the dynamic rupture process and associated radiated seismic energy for faults and simple fault systems that comprise (a) fractally rough fault surfaces and (b) canonical models of segmentation. In part (c), the approaches (a) and (b) are combined to obtain a first-order understanding how small-scale fault roughness may affect rupture-transition properties at segment boundaries. The student will initially test two available HPC-enabled dynamic-rupture simulation codes in terms of performance and for code verification.

Deliverables/Expectations
+ compare two codes/methods using identical numerical parameterization
+ examine rupture process and seismic radiation for various degrees of fault roughness
+ study the rupture jumping (branching vs. jumping) behavior in case of idealized large-scale segmented but small-scale rough faults
+ document results in oral (group-seminar talk) and written (report) form

Field of Study: Geophysics, Seismology

Duration of Internship: 3 months

Temperature of hydrogen-air detonations: Measurements by 2-color planar laser induced fluorescence of the hydroxyl radical

Faculty Mentor
Professor Deanna Lacoste, Mechanical Engineering

Internship Description

Compared to classical constant volume or constant pressure thermodynamic cycles, the detonation regime of combustion could increase by 40% the efficiency of engines. For a long time restricted to military applications, due to the global energetic issue, the civil applications of detonations have received in increasing interest during the last decade. One of the main challenges in this research field is to obtain a self-sustained detonation for practical fuel-oxidizer mixtures (e.g. kerosene-air), in a setup with typical dimensions comparable to those of a commercial gas turbine.
While the quantitative characterization of flames in terms of temperature and chemical species is of current practice, the experimental study of detonation properties is mainly restricted to the determination of the detonation velocity, global pressure, and density gradient structure. Information such as the temperature or density of hydroxyl radical fields in a detonation front have never been measured. However, to better understand the detonation mechanisms and to help in validating detonation models and numerical simulations, these data are crucial.

Objectives: In this context, the main objective of the project is to adapt a non-intrusive thermometry technique broadly used in the combustion community, the 2-color planar laser induced fluorescence on OH, to the characterization of an H2 – air detonation. There are many challenges to obtain reliable temperature measurements of a detonation front, including single shot measurements, synchronization, spectroscopic properties of OH in the condition of the detonation front, etc.

Deliverables/Expectations

First, the student will learn the 2-color PLIF technique on OH in a well characterized configuration: a stable flat flame stabilized over a McKenna burner. During this preliminary step, the uncertainty of the measurements, averaged and single shot, will be characterized. Second, the system will be implemented on a 2D detonation test rig, equipped with optical access for laser diagnostics. One of the main challenges will be the synchronization of the PLIF system with the detonation front arrival in the measurement area. Indeed, the detonation front propagates at a speed of about 2000 m/s, and the jitter between two events in the arrival of the measurement area can be as large as 1 ms. Synchronization will require time of flight measurements and analysis of the detonation propagation front. Finally, post processing of the OH PLIF images will be performed in order to determine the temperature fields. Due to the complexity of the detonation setup and combined laser diagnostics, the experimental part of this study will be performed by two persons: the intern student and an experienced researcher (senior PhD student or post-doc).

Field of Study: Mechanical Engineering, Combustion, Fluid Mechanics **Duration of Internship:** 3 months

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Organic Solvent Nanofiltration

Faculty Mentor

Professor Gyorgy Szekely, Chemical and Biological Engineering

Internship Description

Separation processes play a remarkable role in the chemical and pharmaceutical industries, where they account for 50 to 70% of both capital and operational costs. Organic synthesis in the chemical and pharmaceutical industry are frequently performed in organic solvents and consist of products with high added value that should be removed from the organic solvents. Organic solvent nanofiltration is an emerging technology which allows the isolation and separation of solutes between 50 and 2000 g/mol in organic solvents. The development of nanofiltration membranes stable in harsh environments (e.g. polar aprotic solvents, extreme temperature, pressure and pH) is of utmost importance. Solvent resistant nanofiltration membranes will be fabricated exhibiting superior chemical stability compared to commercial polymeric membranes. The concept of design of experiments (DoE) will be applied throughout the project to gain an in depth understanding parameters governing the membrane will be prepared and crosslinked using aromatic bifunctional crosslinkers. The membrane performance (i.e. flux, retention profile, solvent stability) will be evaluated using a nanofiltration rig.

Deliverables/Expectations

The student will acquire soft skills such as team working, project and time management, giving oral presentations. By the end of the traineeship the student will have a deep understanding of membrane separations, particularly in nanofiltration. Practical and theoretical aspects of surface modification techniques and polymer chemistry techniques will be acquired.

Field of Study: Engineering in Pharmaceutical Industry **Duration of Internship:** 3 months

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Passivation in Perovskite Solar Cells

Faculty Mentor

Professor Stefaan de Wolf, Material Science and Engineering
KAUST Solar Center

Internship Description

Perovskites are an emerging class of materials which offers a high-efficiency photovoltaics owing to its appealing optical and electronic properties. However, defects such as non-coordinated ions at their grain boundaries and surfaces do contribute to non-radiative photo-carrier recombination. This undesirably inflates the open-circuit voltage deficit and is a likely contributor to the widely reported phenomenon of hysteresis in the current-voltage characteristics which is set to remain at the forefront of the continuing progress towards to the theoretical PCE limit of 30%.

In this project, the candidate will have an opportunity to explore some new interfacial engineering strategies, such as surface passivation, grain boundary passivation and contact passivation to eliminate the defects. This will help to increase the open circuit voltage of the perovskite devices which will be employed to achieve champion perovskite/silicon tandem solar cells. At the end of the internship, the candidate(s) will be experienced the full processing steps of the perovskite solar cells and they may have an opportunity to publish the findings in well-respected scientific journals.

Deliverables/Expectations

Exploring new passivation molecules
Testing conductive polymers which has carboxyl groups for passivation purpose
Testing 2D perovskites for interface passivation purpose
Achieving >1.2V open circuit voltage for 1.6 eV perovskite absorbers based solar cells

Field of Study: Solar Cells **Duration of Internship:** 3 months

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Thermal Evaporation of Perovskite Absorbers for Silicon Perovskite Tandem Solar Cells

Faculty Mentor

Professor Stefaan de Wolf, Material Science and Engineering
KAUST Solar Center

Internship Description

Perovskite/silicon tandem solar cells are very promising technology to achieve >30% power conversion efficiency target. Despite this technology features promising efficiency potential, several challenges need to be overcome prior to possible industrial application. A particular challenge relates to the fact that to maximize the light coupling into the bottom cells, the tandems require so-called random-pyramid textured bottom cells (with a feature size of several micron, see Fig. 1a). Whereas flat substrates have enormous reflection losses (Fig. 1c), textured substrates enable improved light coupling into the silicon wafers. Textured silicon solar cells are the industrial state-of-the-art, and there is likely little incentive to develop processes on expensive mirror-polished wafers. However, due to the characteristics of textured surfaces, which present irregularities and low-wetting properties, conventional solution techniques cannot be used to deposit the perovskite or the extraction layers. From this, it can be readily understood that the top cell fabrication needs to rely on scalable and conformal deposition methods, with a high degree of uniformity and reproducibility. For these reasons, we aim in this project to alter our current state-of-the-art solution-based PSC processing procedures as much as possible towards scalable vacuum-based techniques.

In this projects, the candidate will perform an evaporation of perovskites precursors and the conversion of the layers will be performed either by co-evaporation or vacuum/solution hybrid based methods. At the end of the internship period, students will learn how to fabricate and optimize perovskite solar cells. The candidate will have a chance to experience the fabrication of fully textured silicon/perovskite tandem solar cells.
Why thermal evaporated perovskites?
Scalability: vacuum based deposition techniques are a well-established technique in several industrial processes.
Reproducibility: thermal evaporation process of perovskite absorbers is not affected by the multitude of uncontrollable parameters typical for solution-processed perovskites.
Uniformity: unlikely solution deposition, evaporation enables uniform deposition, independently from the substrate type.
Low thermal budget: thermal evaporation is a low-temperature process and the substrate can be eventually further cooled to room temperature.
Environmentally benign: evaporation does not involve toxic solvents.
Process flexibility: different perovskite composition can be obtained by evaporation, according to the desired application.

Deliverables/Expectations

Thickness control of the evaporated lead iodide
Optimization of co-evaporated of lead iodide and cesium bromide
Process sophistication for triple cation system perovskites
>23% tandem solar cell efficiency using thermal evaporated perovskites

Field of Study: Solar Cells **Duration of Internship:** 3 months

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Broadband Transparent Front Electrodes for Perovskite Silicon Tandem Solar Cells

Faculty Mentor

Professor Stefaan de Wolf, Material Science and Engineering
KAUST Solar Center

Internship Description

This project is focusing on developing novel transparent electrodes for perovskite/silicon tandem solar cells which are an emerging class of solar cells technology. Perovskite/silicon tandem solar cells aim to achieve the power conversion efficiencies beyond the single junction limit of the silicon solar cells. Towards this end, developing highly transparent electrodes are critical for the maximized light harvesting since parasitic absorption loses originating from the transparent conductive oxides causes drastic current losses.

In this project, the deposition of the novel transparent conductive oxides will be performed the sputtering technique. The candidate will gain experience on the structural, optical and electrical and characterization of the thin films. Moreover, the candidate will have experience in the fabrication and characterization of the perovskite/silicon tandem solar cells to test the developed materials.

Why we need broadband transparent electrodes on perovskite/silicon tandem solar cells?
In perovskite/silicon tandem solar cells, the perovskite top cell efficiently harvests the blue part of the solar spectrum, while transmitting the red part, which is absorbed in the silicon bottom cell. In this way, the tandems can overcome the single-junction efficiency limit of silicon solar cells. However, parasitic absorption losses originating from the transparent electrodes hinders the light harvesting. Typically, a front transparent electrode in any solar cell has a sufficiently large (>3 eV) optical band gap to avoid absorption losses in the visible range of the spectrum. This requirement is already fulfilled by several TCOs such as ITO, IZO, and IO: H. For perovskite/silicon tandem solar cells, transparent electrodes with low absorptance in the NIR-IR part of the spectrum are required since these devices use optical absorbers that are active in this range of the spectrum. Towards reaching >30% photoconversion efficiency, designing transparent electrodes with exceptionally large broadband transparency carriers critical importance.

References
[1] Morales-Masis, M., De Wolf, S., Woods-Robinson, R., Ager, J. W., & Ballif, C. (2017). Transparent electrodes for efficient optoelectronics. Advanced Electronic Materials, 3(5), 1600529.

Deliverables/Expectations
Optimization of the sputtering parameters of H:In2O3 and IZO transparent electrodes
Optical and electrical characterization of the fabricated films
Achieving <20 ohm/sq. sheet resistivity for 1000 nm thickness together with broadband transparency (<10% absorbance within this region).
Exploring new TCO by metal doping of In2O3

Field of Study: Solar Cells **Duration of Internship:** 3 months

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Novel Electron and Hole Transport Layers by Atomic Layer Deposition Technique for Perovskite Silicon Tandem Solar Cells

Faculty Mentor

Professor Stefaan de Wolf, Material Science and Engineering
KAUST Solar Center

Internship Description

The atomic layer deposition (ALD) technique is an efficient technique to deposit thin films at low temperature, which is based on self-limiting surface reactions by exposing sequentially on the substrate with various precursors and reactants. It provides excellent control over film thickness at the angstrom or monolayer level and deposition on high aspect ratio nano and microstructures with excellent step coverage. To exploit these advantages, we are employing ALD deposited electron and hole transport layers on randomly textured silicon wafers.

In this project, to increase the light coupling in the tandem solar cells, the deposition of the broadband transparent electron and hole transport layers will be performed by the ALD technique. The candidate will gain experience on the structural, optical and electrical and characterization of the thin films by optimizing the deposition recipes. Moreover, the candidate will have experience in the fabrication and characterization of the perovskite solar cells and will have an opportunity to experience the fabrication of perovskite/silicon tandem solar cells.

Why Silicon/Perovskite Tandems?

The current global photovoltaics market (nowadays taken for more than 90% by crystalline silicon solar cells) has seen a sustained growth of its production capacity by more than 20% annually [1]. From a longer-term perspective, the market is expected to make a transition towards ultra-high efficiencies. For this, further efficiency improvement s will be needed, beyond the single-junction efficiency limit of silicon [2]. The most straight-forward way to do so is in the form of a silicon-based tandem solar cell, where a wider-bandgap top cell overlays the silicon bottom cell.

In perovskite/silicon tandem solar cells, the perovskite top cell efficiently harvests the blue part of the solar spectrum, while transmitting the red part, which is absorbed in the silicon bottom cell. In this way, the tandems can overcome the single-junction efficiency limit of silicon solar cells.

References

[1] Haegel, Nancy M., et al. "Terawatt-scale photovoltaics: Trajectories and challenges." Science 356.6334 (2017): 141-143.

[2] Richter, A., Hermle, M., & Glunz, S. W. (2013). "Reassessment of the limiting efficiency for crystalline silicon solar cells." IEEE Journal of Photovoltaics, 3(4), 1184-1191.

Deliverables/Expectations

Optimization of SnO_2 thin films for perovskite solar cells applications

Testing these layer for flat junction opaque devices for performance analysis

Achieving >23% tandem solar cells efficiency using these buffer layers.

Testing new ALD precursors for electron and hole transporting purposes

Field of Study: Solar Cells **Duration of Internship:** 3 months

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In-liquid Visualization of Phenol during Plasma Purification

Faculty Mentor

Professor Min Suk Cha, Mechanical Engineering
Clean Combustion Center

Internship Description

In-liquid plasma generation is of interest topic due to intrinsic physics behind as well as a wide range of applications. This project consists of in-water electrical discharges with gas bubbles to investigate a degradation of phenol as a model contaminant. Particularly, a laser induced fluorescence will be adopted to visualize a spatial distribution of phenol when it is being decomposed.

Deliverables/Expectations

Cross sectional imaging of phenol distribution with bubbles in water and Submission to a peer reviewed journal

Field of Study: Mechanical Engineering **Duration of Internship:** 3 months

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Investigation of nanoparticulate morphology at PPC and HCCI modes

Faculty Mentor

Professor Bengt Johansson, Mechanical Engineering
Clean Combustion Center

Internship Description

1. A thermophoretic probe will be designed for soot collection from engines exhaust pipe.
2. The nanoparticulate will be collected for morphology from different combustion mode, like HCCI, PPC, and CI.
3. The distribution of particle size and number density will be investigated.
4. The low octane number fuel, naphtha, will be fueled with the compression ignition engine to investigate the nanoparticulate emissions

Deliverables/Expectations

1.A thermophoretic probe. 2. Nanoparticulate TEM and HR-TEM images
2. Journal papers, like Combustion and Flame or Applied energy

Field of Study: Combustion engine and nanoparticulate emissions **Duration of Internship:** 3 months

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Modeling structure and properties of transition metal complexes

Faculty Mentor
Professor Luigi Cavallo, Chemical Science
Catalysis Center

Internship Description
This project is focused on the characterization of transition metal based catalysts using quantum mechanics approaches. The applicant will have to correlate the experimental behavior of families of catalysts based on a transition metal to the structure of the ligand coordinated to the metal using molecular descriptors.

Deliverables/Expectations
A scientific report summarizing the results of the research

Field of Study: Computational chemistry; catalysis. **Duration of Internship:** 3 months

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Applications of reduced graphene oxide

Faculty Mentor
Professor Pedro Da Costa, Material Science & Engineering
Laboratory for Carbon Nanostructures

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.

Field of Study: Chemistry / Materials Science / Physics **Duration of Internship:** 3 months

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Future Fuel for Advanced Combustion Engines

Faculty Mentor
Professor Aamir Farooq, Mechanical Engineering
Chemical Kinetics and Laser Sensors Laboratory

Internship Description
Increasing focus on global warming and CO2 emsisions 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 CO2 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
Perofrm 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.

Field of Study: Mechanical Engineering, Chemical Engineering, Chemistry
Duration of Internship: 3 months

Big Data: Mess versus Value

Faculty Mentor
Professor Tedeusz Patzek, Energy Resources and Petroleum Engineering
Petroleum Engineering Research Center

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.

Field of Study: Drilling, production, or reservoir engineering. **Duration of Internship:** 3 months

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Expression, Purification, Characterization of Proteins for Biocatalysis

Faculty Mentor
Professor Magnus Rueping, Chemical Science
Catalysis center

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. These new metalloproteins possess reactivities nature does not provide. The further goal will be the examination of the new metalloprotein in aqueous catalysis reactions and the examination of the influence of further mutations on selectivity and reactivity.
Project-duration will be 3-6 month, details of arrival/departure dates to be discussed.

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.

Field of Study: Chemistry/Biochemistry/Molecular Biology **Duration of Internship:** 3 months

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Functionalization of Gas Vesicles

Faculty Mentor
Professor Magnus Rueping, Chemical Science
Catalysis center

Internship Description
Engineered Gas Vesicles are tailor-made for purposeful catalysis platform. Now these engineered Gas Vesicle shall be tested for thermal, salt and solvent stability. Further, these functionalized gas vesicles will be tested in aqueous catalysis reactions and the influence of different functionalization strategies on selectivity and reactivity will be studied.
Project-duration will be 3-6 month, details of arrival/departure dates to be discussed.

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.

Field of Study: Chemistry/Biochemistry/Molecular Biology **Duration of Internship:** 3 months

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Visible-light Photoredox Catalysis Transformations

Faculty Mentor
Professor Magnus Rueping, Chemical Science
Catalysis center

Internship Description
The use of sun-light in organic transformations allows the development of sustainable transformations. Several new visible-light exited photocatalysts and polymers have been prepared. These new catalytic materials will be tested in photochemical processes including new bond formations.
Project-duration will be 3-6 month, details of arrival/departure dates to be discussed.

Deliverables/Expectations
Students shall extend their general knowledge and skills in organic chemistry and catalysis. An emphasis will be put on the synthesis and application of new photocatalysts. 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 a final written report.

Field of Study: Chemistry/Biochemistry/Molecular Biology **Duration of Internship:** 3 months

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High Pressure Heterogeneous Autoignition of Hydrocarbon and Syngas Fuels

Faculty Mentor
Professor William Roberts, Mechanical Engineering
Clean Combustion Research Center

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

Field of Study: Mechanical Engineering, Chemical Engineering, Aerospace Engineering, Physics.
Duration of Internship: 4 to 6 months

Engineering Chemical Reactions with Machine Learning

Faculty Mentor
Professor Mani Sarathy, Chemical and Biological Engineering
Clean Combustion Research Center

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.

Field of Study: Computer Science, Computer Engineering, Software Engineering, Chemical Engineering
Duration of Internship: 3 months

First-principles investigation of superlattices of 2D materials

Faculty Mentor
Professor Udo Schwingenschlogl, Material Science & Engineering
Computational Physics & Material Science

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.
Field of Study: Computational Materials Science **Duration of Internship:** 3 months

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Dynamics of MEMS for mechanical computing

Faculty Mentor
Professor Mohammad Younis, Mechanical Engineering
Nano/Micro Mechanics and Motion (NM3) Laboratory

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.

Field of Study: Mechanical engineering **Duration of Internship:** 3 months

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Simulations of Large Scale Turbulent Flames using OpenFOAM

Faculty Mentor
Professor Hong Im, Mechanical Engineering
Clean Combustion Center

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.

Field of Study: Mechanical/Aerospace/Chemical Engineering, Applied Physics/Mathematics
Duration of Internship: 3 months

Simulations of Spray and Combustion in Engines

Faculty Mentor

Professor Hong Im, Mechanical Engineering
Clean Combustion Center

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.

Field of Study: Mechanical/Aerospace/Chemical Engineering, Applied Physics/Mathematics
Duration of Internship: 3 months

New Materials and Process for High Performance Organic Solar Cells

Faculty Mentor

Professor Iain McCulloch, Chemical Science
Solar Center

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.

Field of Study: Chemistry **Duration of Internship:** 3 months

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Novel highly efficient hole transporting layers for perovskite solar cells

Faculty Mentor

Professor Iain McCulloch, Chemical Science
Solar Center

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.

Field of Study: Material Science and Engineering, Applied Physics, Chemistry
Duration of Internship: 3 months

Development of Water-Soluble Semiconducting Polymers for Organic Bioelectronic Devices

Faculty Mentor
Professor Iain McCulloch, Chemical Science
Solar Center

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.

Field of Study: Biophysics, Physics, Chemistry, Material Science **Duration of Internship:** 3 months

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Chemical Kinetics of Novel Biofuels

Faculty Mentor
Professor Aamir Farooq, Mechanical Engineering
Chemical Kinetics and Laser Sensors Laboratory

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

Field of Study: Mechanical Engineering or Chemical Engineering **Duration of Internship:** 3 months

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Novel Phenomena at perovskite interfaces and superlattices

Faculty Mentor

Professor Udo Schwingenschlogl, Material Science & Engineering
Computational Physics & Material Science

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 $LaAlO_3$ and $SrTiO_3$, 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

Field of Study: Physics, Materials Science, Chemistry, Electrical Engineering
Duration of Internship: 3 months

Role of non-classical hydrogen bonding in organocatalysis

Faculty Mentor
Professor Kuo Wei (Andy) Wang, Chemical Science
Catalysis center

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.

Field of Study: Chemistry **Duration of Internship:** 3 months

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First principles modeling of hybrid organic-inorganic perovskites

Faculty Mentor
Professor Udo Schwingenschlogl, Material Science & Engineering
Computational Physics & Material Science

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 $MAPbI_3$ perovskite (MA= Methylammonium = $CH_3NH_3^+$) 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 $MAPbI_3$ 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.

Field of Study: Physics, Materials Science, Chemistry, Electrical Engineering
Duration of Internship: 3 months

Adhesion phenomena across interfaces with spatially heterogeneous adhesive properties

Faculty Mentor
Professor Gilles Lubineau, Mechanical Engineering
Composite and Heterogeneous Material Analysis and Simulation Laboratory

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.

Field of Study: Mechanical engineering. Material science, civil engineering
Duration of Internship: 3 months

Ultra Sensitive Sensors based on Nanotubes Porous Networks

Faculty Mentor
Professor Gilles Lubineau, Mechanical Engineering
Composite and Heterogeneous Material Analysis and Simulation Laboratory

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.

Field of Study: Mechanical Engineering **Duration of Internship:** 3 months

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Mechanical properties of new integrated flexible electronics based on doped thermoplastics

Faculty Mentor
Professor Gilles Lubineau, Mechanical Engineering
Composite and Heterogeneous Material Analysis and Simulation Laboratory

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 prooerties 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.

Field of Study: Mechanical Engineering **Duration of Internship:** 3 months

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Mechanical integrity of thermoplastics structural composites

Faculty Mentor
Professor Gilles Lubineau, Mechanical Engineering
Composite and Heterogeneous Material Analysis and Simulation Laboratory

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 inolved 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.

Field of Study: Mechanical Engineering **Duration of Internship:** 3 months

Experiments on High-Speed Multi-Phase Flow

Faculty Mentor
Professor Sigurdur Thorodsen, Mechanical Engineering
HIgh-Speed Fluids Imaging Laboratory

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.The results are utilized for publications.

Field of Study: Fluid Mechanics, Mechanical Engineering or Chemical Engineering
Duration of Internship: 3 months

Monitoring subsidence due to groundwater pumping in central Arabiaxperiments on High-Speed Multi-Phase Flow

Faculty Mentor
Professor Sigurjon Jonsson, Earth Science and Engineering
Crustal Deformation and InSAR Group

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.

Field of Study: Earth Science, Environmental science and engineering
Duration of Internship: 3 months

Constraining Earth Fluid Motion Models with Satellite Images

Faculty Mentors

Professor Ibrahim Hoteit, Earth Science and Engineering, Earth Fluid Modeling & Prediction
Professor Ganesh Sundaramoorthi, Visual Computing Science

Internship Description

Developing exact mathematical models to stimulate and predict oceanic and atmospheric motions is a difficult process because of the complex multi-physical intereactions. Satellite images provide a powerful tool to extract in detail some information at various scales that could be used to reduce the uncertainies 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 contraining 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 flitering methods for images assimilation. Implement and assess performance with numberical test models (e.g. Shallow water)

Field of Study: Applied Mathematics, Earth Sciences and Engineering, Electric Engineering or any related field
Duration of Internship: 3 months

Wafer-scale patterned growth of vertically aligned carbon nanotubes

Faculty Mentor

Professor Pedro Da Costa, Material Science & Engineering
Laboratory for Carbon Nanostructures

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

Field of Study: Materials Science and Engineering / Chemistry / Physics
Duration of Internship: 3 months

Direct Numerical Simulation of Turbulent Combustion at High Pressures

Faculty Mentor
Professor Hong Im, Mechanical Engineering
Clean Combustion Center

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.

Field of Study: Mechanical/Aerospace/Chemical Engineering, Applied Physics/Mathematics
Duration of Internship: 3 months

Fuel Design

Faculty Mentor
Professor Mani Sarathy, Chemical and Biological Engineering
Clean Combustion Research Center

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.

Field of Study: Chemical Engineering, Mechanical Engineering, Chemistry **Duration of Internship:** 3 months

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Quantifying and reducing uncertainties in earth fluid models

Faculty Mentors
Professor Ibrahim Hoteit, Earth Science and Engineering, Earth Fluid Modeling & Prediction
Professor Omar Knio, Applied Mathematics and Computational Science

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.

Field of Study: Applied Mathematics, Earth Sciences and Engineering, or any related field
Duration of Internship: 3 months

Synthesis of Novel Pincer complexes

Professor Kuo Wei (Andy) Wang, Chemical Science
Catalysis center

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 trained on standard organic synthesis knowledge and Schlenk skills.

Field of Study: Chemistry **Duration of Internship:** 3 months

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Enhancing Weather Downscaling and Forecasting

Professor Ibrahim Hoteit, Earth Science and Engineering, Earth Fluid Modeling & Prediction

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.

Field of Study
Applied Mathematics, Meteorology, or any related field **Duration of Internship:** 3 months

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Experimental study of carbon-free combustion

Faculty Mentor
Gaetano Magnotti, Mechanical Engineering
Clean Combustion Research Center

Internship Description
A major goal of combustion research is to reduce emissions and minimize the harmful impact of energy production and transportation on the environment. Advancements in combustion sciences enabled strong reduction of NOX, SOX and particulates. The challenge for the next decade is reduction of carbon dioxide. One strategy is to completely remove carbon from the fuel, using carbon-free hydrogen carrier such as ammonia. Combustion of ammonia is not well understood, and no detailed information on the flame of ammonia-air flames is available. In this project the student will perform 1D Raman measurements of temperature and major species in ammonia flames in collaboration with a postdoc or a Ph.D. student.
Deliverables/Expectations
The student will learn the fundamental of laser spectroscopy, and will gain hands-on experience in the operation of ammonia burners, and advanced laser diagnostics. He will acquire and analyze unique experimental datasets, and advance the understanding of combustion of ammonia-air flames.

Field of Study **Duration of Internship:** 3 months

Mechanical, Aerospace, Chemical Engineering or Applied Physics