Online Proceedings

Poster Session 1

Commons East, Easel 68

11:00 AM to 1:00 PM

Image Analysis for Automation of Labeling Multivariate AFM Images of Coherent Bio-Nano Interfaces for Machine Learning Applications

Erik Matthew Johnson, Senior, Materials Science & Engineering
Jack Otto Ryan, Junior, Pre Engineering
Mentor: Siddharth Rath, Materials science and engineering, Genetically Engineered Materials Science and Engineering Center
Mentor: Mehmet Sarikaya, Materials Science & Engineering

Atomic Force Microscopy (AFM) images of peptide self-assembly on two dimensional atomically-thin inorganic solid substrates have features that are difficult to extract because of the diverse conformations these peptides have on the surfaces from nanoislands, no nanowires to confluent films and disorganized nanostructures. Analysis of these images can produce parameters such as thickness, aspect ratio, order/disorder ratio, and orientation distributions quickly and accurately. The first step is to input data in a table and convert it into an array. The images are then converted into a grayscale version, its background noise subtracted and subsequently renormalized. User determined edge detection techniques are then used to delineate the edges in the images. Appropriate segmentation methods are then used to separate different types of nanostructural textures and phases, and coupled with the edge information. Several further parameters such as percent area and volume fraction of each phase (surface coverage), percent-ordering in the long-range ordered phases, their shape and orientation distributions, as well as relative sizes are identified and quantified from the images. The sets of unique parameter are then used as the bases for assigning specific labels for the degree of molecular recognition of the substrate by the peptides and eventual orientation relationships between the peptide nanostructures and the crystalline lattices of the 2D atomically thin solid substrates. These labels are then used to train a machine learning algorithm to cluster these images and relate them to processing parameters associated with them via a relational database. The eventual goal here is to parameterize the images so that we can predict the ordering characteristics of any peptide-substrate pair to accelerate design of future technologies, e.g., bionanosensors, emanating from these hybrid material systems.

Poster Session 2

MGH 241, Easel 155

1:00 PM to 2:30 PM

Towards Biomimetic Treatment of Gum Disease: Repair of PDL via Peptide-guided Remineralization

Keertana Krishnan, Senior, Materials Science & Engineering
UW Honors Program
Yousef Mohammed Baioumy, Junior, Chemical Engineering
Mentor: Mehmet Sarikaya, Materials Science & Engineering
Mentor: Deniz Tanil Yucesoy, Materials Science and Engineering
Mentor: Sanaz Saadat, Oral Health Sciences
Mentor: Sami Dogan, Restorative Dentistry

Periodontal disease (PDL) results from a serious infection in the gingival tissue (gum) that can eventually lead to tooth loss and jawbone damage. The disease is common with more than 3 million cases in the US per annum. Bacteria build up in plaque lead to gingivitis and periodontitis under improper oral hygiene. If left untreated, the supporting tissues of the teeth e.g., cementum and periodontal ligaments will be lost, therefore making the teeth and supporting tissues vulnerable to bacterial attack, leading to serious infections and, even, to death. Current approaches in regenerating periodontal ligaments include the use of bioactive molecules and barrier membranes for guided tissue regeneration using human stem cells. Although the utilization of such materials enhances the cell proliferation and differentiation to a degree, the absence of cementum-like tissue prevents the complete regeneration of periodontal ligaments on the tooth surface. The aim of this project is to develop a biomimetic strategy to restore cementum tissue and regenerate the periodontal ligaments using human periodontal ligament (hPDL) cells in vitro. Using peptide-guided remineralization, we created a new cementum-like mineral layer on exposed dentin. The hPDL cells are then cultured and seeded on the novel cemento-mimetic layer and induced to differentiate. The proliferation and differentiation of the hPDL cells are monitored in detail using 3-(4,5-Dimethylthiazol-2-yl)-

2,5-diphenyltetrazolium bromide (MTT) and alkaline phosphatase (ALP) assays, respectively. Our results show that the newly formed cemento-mimetic mineral layer facilitates the hPDL growth and differentiation. The method described herein offers a unique biomimetic solution to regenerate periodontal ligaments and thereby ultimately prevent tooth loss and eliminate periodontal disease. This work is supported by WA-State Life Sciences Discovery Funds, UW-School of Dentistry Spencer Funds, and Amazon-UW/CoMotion Catalyst Program.

POSTER SESSION 4

Commons West, Easel 23

4:00 PM to 6:00 PM

An Early-Stage Pancreatic Cancer Diagnostic: Fabrication of a Graphene Field-Effect Transistor Utilizing a Modular Chimeric Probe Assembly for Biomarker Detection

Rebeka Khajehpour, Senior, Physics: Applied Physics
Jessica Elise Ahrens Tran, Senior, Materials Science & Engineering
Zane Prior Smith, Senior, Physics: Biophysics, Gender, Women, and Sexuality Studies
UW Honors Program
Mentor: Richard Lee, Materials Science & Engineering
Mentor: Mehmet Sarikaya, Materials Science & Engineering
Mentor: David Starkebaum, MSE

The goal of our project is to create an electronic device capable of early detection of pancreatic cancer (PC) with high selectivity and sensitivity. PC projects a very low survival rate often due to late-stage cancer diagnosis. Recent research has established that there are PC biomarkers prevalent throughout the body for several years before symptoms emerge. The consequent wider time window presents an opportunity for these biomarkers to be detected at their initial low concentrations thus allowing for early diagnosis. Our device uses a modular sensing construct consisting of an immobilized probe molecularly bound to the surface of the sensor device. Detection occurs when a target biomarker specifically binds to the probe and changes the electrical properties of the sensing surface that is measured quantitatively. Validating the functionality of the sensing construct and its properties is accomplished through a variety of molecular adsorption and binding techniques that assess each step; from probe immobilization to target detection. Using this modular design, research is underway to develop an array of sensors, thus potentially revolutionizing rapid medical diagnostics to provide long-term health monitoring of PC and other cancers.

POSTER SESSION 4

MGH 206, Easel 172

4:00 PM to 6:00 PM

Engineering a Peptide-Guided Biomimetic Treatment for Dental Hypersensitivity

Eric Linden Hall, Senior, Materials Science & Engineering
Andrea Ming Hwei Dao, Senior, Chemical Engineering
Saleh Abdullatif S Alhamad, Junior, Bioresource Science and Engr: Business
Mentor: Mehmet Sarikaya, Materials Science & Engineering
Mentor: Deniz Tanil Yucesoy, Materials Science and Engineering
Mentor: Hanson Fong, Materials Science & Engineering
Mentor: Sami Dogan, Restorative Dentistry

Dental hypersensitivity (DH) is a common oral health condition in the U.S. affecting the majority of the adult population. It is caused by the exposure of dentin due to the demineralization of the protective cementum or enamel that covers the tooth surface. When the dentinal tubules are exposed, nerve fibers in the pulp or predentin are stimulated by the displacement of the fluid and report pain. The stimulus that triggers the onset of pain can be of thermal, chemical or mechanical origin. There is still no effective agent to completely resolve the patient's discomfort with DH. Over-the-counter products are commonly advised in the management of DH while toothpastes containing strontium, oxalate or potassium salts, or fluoride are recommended with limited efficacy to reduce the sensitivity from DH. Restorative materials using composite, glass ionomer or amalgam are adapted to treat the affected area with limited success. The goal of this project has been to develop a biomimetic treatment by restoring cementum tissue using a peptide-guided remineralization approach, thereby occluding the exposed tubules with a newly formed mechanically and thermally stable mineral layer. The College of Engineering working closely with School of Dentistry-UW involves mimicking the hypersensitivity condition by removing enamel/cementum of extracted human teeth to expose underlying dentin. The samples are then treated with peptide-guided remineralization resulting in 10+ micrometer thick new layer over the damaged dentin. Our results exhibit a highly effective way to occlude the exposed dentinal tubules by a newly formed mineral layer which penetrates into the dentin tubules. The method described herein offers a unique biomimetic treatment protocol for dental hypersensitivity, which will be developed as a platform technology for effective in-clinic and over-the-counter hypersensitivity treatments. The work is supported by WA-State Life Sciences Discovery Funds, UW-School of Dentistry Spencer Funds, and Amazon-UW/CoMotion Catalyst Program.

Poster Session 4

MGH 206, Easel 173

4:00 PM to 6:00 PM

Effective Utilization of Experimental and Modeling Data in Innovation via Machine Learning, Data Analytics, and AI: Looking inside the Black Box

John Taylor (John) Hamann, Senior, Mechanical Engineering
Jack Otto Ryan, Junior, Pre Engineering
Benjamin (Ben) Mac Millan, Sophomore, Pre-Sciences
Antonio R. Crowe, Junior, Chemistry, Materials Science & Engineering
Mentor: Mehmet Sarikaya, Materials Science & Engineering
Mentor: Siddharth Rath, Materials science and engineering, Genetically Engineered Materials Science and Engineering Center
Mentor: Burak Berk Ustundag, Materials Science and Engineering
Mentor: David Starkebaum, MSE

In scientific research labs, in general, experiments are generally treated as a black box: a prepared sample goes in, something happens, and one gets results that are then obtained via elaborate characterization steps. Several important dependent or correlated parameters are either discarded or ignored because of a lack of coherent dependency analyses that require critical thinking, linking, and pattern recognition. In this research we are working to stop treating experiments and computational simulations as black boxes, and create a cohesive platform where materials used, processes and parameters utilized and results achieved can be brought together as separate but related sets of databases. In the next step, the relationships between all the different parameters can then be connected, analyzed and visualized. Machine learning and AI techniques can then be used to predict results using these databases, thereby reducing experiment time, and taking away the traditional 'trial and error' method of experimentation. The research involves creation of a software interface, with numerous image and signal processing tools and applications running on libraries made customizable to research fields, types of experiments, etc. Assorted variety of services such as parallelization, compression, data analysis, and visualization, caching (among others) are also provided. We are improving the accuracy of time series data analysis and using fingerprinting to depict all parameters for improved predictability, flexibility and accuracy. When fully developed, we anticipate that the program will enable experimental and computational researchers to extensively use, customize and apply data analytics, machine learning and AI even in niche research in the hard sciences at the intersection of biology and genetics, materials science (physics, chemistry) and engineering, and computational modeling and informatics, enabling faster and accurate cross disciplinary innovation in technology and medicine. The research is supported by NSF-DMREF (DMR-1629071) program at GEMSEC-MSE, as part of National Materials Genome Initiative.

Poster Session 4

Commons West, Easel 25

4:00 PM to 6:00 PM

Bridging Biology with Solid-State Devices: Molecular Phase Behavior of Self-Assembled Peptides on 2D Atomic Layered Materials

Madelyn Joy Milligan, Senior, Materials Science & Engineering
Tyler Scott Chinn, Senior, Materials Science & Engineering
Mentor: Ty Jorgenson
Mentor: Mehmet Sarikaya, Materials Science & Engineering

A strategic area of focus in the field of molecular biomimetics integrates biology and inorganic materials to create novel bioelectronic devices. Using combinatorial mutagenesis, the GEMSEC lab at UW has developed genetically engineered peptides for inorganics (GEPIs) consisting of short (˜12 amino acids) sequences that specifically bind to solid state materials (i.e. graphite, MoS2, BN). This binding specificity allows for seamless integration between biological and solid substrates, uniquely bridging the worlds of biology and solid state devices. The structure of the bio/nano interface in these systems has profound impacts on the subsequent device properties, performance, and durability. Therefore it is important to understand how the processing conditions affect the structure – a cornerstone of materials science and engineering. To this end, we aim to develop a phase diagram that will allow for quantitative prediction of the bio/nano interface's self-assembled structure. The peptide is deposited in solution onto a graphite surface, incubated under specifically defined experimental conditions, then examined using atomic force microscopy (AFM). Herein, we investigate the effects of experimental conditions (peptide concentration, incubation temperature, and electrochemical bias/pH) on the peptide's assembled structure on 2D layered materials. These fundamental parameters are essential to elucidate the kinetics and thermodynamics of the molecular assembly process allowing for further design, engineering, and coding of the processes of these hybrid materials systems, providing the much needed fundamental science toward biology-guided solid state devices.

Poster Session 4

Commons West, Easel 17

4:00 PM to 6:00 PM

Peptide-Enabled Fluorescent *in situ* Identification of Phytoliths in Contemporary Plants

Gwendolyn Joanna (Gwen) Xiao, Junior, Pre-Sciences
Mentor: Mehmet Sarikaya, Materials Science & Engineering
Mentor: Deniz Tanil Yucesoy, Materials Science and Engineering
Mentor: Caroline Stromberg, Biology

Phytoliths are microscopic silica bodies that form in many plants. Being resistant to organic decomposition, they can be used to track plant evolution and past vegetation changes. Although they were traditionally considered as non-functional cellular by-products, recent studies suggest that phytoliths may have photonic, structural, nutritional and defensive benefits in plant growth and survival. Grasses, which are large terrestrial producers of biogenic silica, are the suitable model system for studying the adaptive significance of silica accumulation in plants. Identification of phytoliths within the plants (for studying function) and inside the sediments (for studying evolution of vegetation) have so far been limited to optical microscopy-based methods where fluorescent dyes are commonly used to increase contrast between silica bodies and plant tissue. Due to their non-specific nature, however, fluorescent dyes often accumulate in different parts of the cells and silicified tissues, causing false positives and leading to incomplete staining and difficulties to construct 3D structures. With exquisite molecular recognition and assembly properties, solid-binding peptide tags (dubbed GEPIs) are surface functionalization moieties that can be chimerized with fluorescent and utilized as material-specific probes to selectively label variety of inorganic materials at surfaces and within interfaces. Our goal is to develop peptide-based phytolith-specific fluorescent probes to identify and delineate phytolith shapes with high precision and *in situ*. Using phytoliths-specific peptides probes, designed and chimerized with fluorescent molecules, our goal is to incubate different grass species, and visualize them using laser-confocal microscopy. We hypothesize that the novel molecular construct enable specific detection of phytoliths *in situ*. The method we are developing will offer a unique solution for fast and accurate identification and 3D organization of inorganic nano- and micro-structures in tissues from living plants and in paleontological samples.