

Siemens Competition

Math : Science : Technology

Regional Finalist

Names: Ketan Agrawal and Hari Kothapalli

High School: Columbus Academy and Roxbury Latin School

Mentor: Dr. Miriam Rafailovich

Project Title: *Enhancing the Efficiency of Bulk Heterojunction Solar Cells Via the Addition of Amorphous and Semicrystalline Nanostructuring Polymers*

Previous studies have shown that the addition of non-photoactive polymers into the active layer of bulk heterojunction (BHJ) solar cells can improve efficiency by structuring columnar domains that decrease the path length to the electrode.^{1,2} Here, we test power conversion efficiency (PCE) of BHJ solar cells based on the polymer donor poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)] (PCDTBT) and the fullerene acceptor [6,6]-phenyl-C61-butyric-acid-methyl-ester (PC₆₀BM,) as well as an inert polymer: either the amorphous copolymer poly(styrene-co-acrylonitrile) (SAN) or the semicrystalline thermoplastic poly(lactic acid) (PLA,) the latter of which is a novel blending component in BHJ solar cells. While SAN:PCDTBT:PCBM and PLA:PCDTBT:PCBM blends at the 4:4:16 ratio displayed poor average PCEs relative to the 4:16 PCDTBT:PCBM control, reducing the blending ratio to 1:4:16 for both blends led to enhanced PCEs of 2.75% and 2.82%, representing 19.6% and 22.1% increases over the control, respectively. Reducing the blending ratio also transformed the thin-film morphology of the solar cells from large, bicontinuous phases at 4:4:16 to interpenetrating, column-like domains at 1:4:16, which creates pathways for charge transport and optimizes exciton dissociation. These results suggest that tuning the blending ratio, rather than chemical composition of non-photoactive polymers, is paramount to controlling morphology and enhancing efficiency.

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Regional Finalist

Names: Katherine Cao, Alice Wu, & William Hu

High School: Homestead High School, Half Hollow Hills High School West, & Saratoga High School

Mentors: Miriam Rafailovich & Adriana Pinkas-Sarafova, Stony Brook University

Project Title: *Characterizing Novel, Spun-Cast PLA/Polystyrene Substrates of Differential Nanoscale Surface Topographies and Optimizing Cell-Plating Density to Promote Dental Pulp Stem Cell Proliferation and Differentiation in vitro*

Dental pulp stem cells (DPSCs) hold tremendous potential in tissue and bone regeneration on in vitro substrates. This study evaluated the effects of nanoscale surface topography and cell-plating density on DPSC proliferation and differentiation. Polylactic acid (PLA), a highly biocompatible polymer, was spun-cast with polystyrene (PS) onto silicon wafers. The PS was removed through dissolution to construct varying surface topographies, before DPSCs were plated onto the substrates to study cell behavior. While bi-polymer blends have been studied in previous experiments, our technique in the creation of polymer thin film surfaces is novel. Atomic force microscopy was used to characterize the surfaces and confocal microscopy revealed the favorable spreading of actin filaments over porous surfaces. Based on early-stage proliferation, higher cell-plating densities were found to correspond with higher plating efficiencies. Scanning electron microscopy verified the biomineralization of the cells, and real-time polymerase chain reaction analysis identified the various differentiation markers of the DPSCs. All surfaces were able to induce biomineralization; however, the PLA-MG 1:PS(45.8K) 1 surface induced the most osteogenic differentiation, likely due to its similarity to dentin. The implications of our findings hold promise in the field of regenerative medicine.

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Regional Finalist

Names: Dhweeja Dasarathy

High School: Hawken School

Mentor: Yoichiro Ito

Project Title: Novel column designs for improved bioseparation of complex molecules using counter current chromatography

Despite major advances in detection methods, bioseparation limits molecular discoveries. Countercurrent chromatography (CCC) is a liquid-liquid partition chromatography that uses the Archimedean Screw principle to significantly decrease sample loss and denaturation by eliminating a solid support matrix. However, loss of stationary phase and consequent sample loss has not been eliminated. A novel flat spiral tube assembly was made based on the forces generated and calculated partition coefficients. Separation of mixtures of cytochrome c, hemoglobin, myoglobin, ovalbumin, and lysozyme proteins showed that partitioning efficiency was significantly enhanced with the new flat-tube compared with conventional columns. A novel tube modifier was then used to generate columns with varying internal diameters and shapes. Column performance measured by theoretical plate number, peak resolution, stationary phase retention, and separation time showed significantly enhanced performance efficiency for our new flat-tube column. Column and tube tolerance of large forces limited revolution speeds and resulted in longer run times. Improvement in separation efficiency and shorten run times, especially for large molecules was achieved with a thin layer CCC using a plastic disc. Modifications of CCC columns based on structural properties of the tubes and the forces generated results in enhanced bioseparation efficiency that has broad applications in science.

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Regional Finalist

Names: Shivani Konduru, Sara Huang, and Tiffany Guo

High School: Troy High School, Troy, MI

Mentor: Dr. James Huang

Project Title: *The Mechanism and Diagnostic Significance of Surface Immunoglobulin Light Chain Negative Mature B-Cells* (Biology)

Surface immunoglobulin light chains are not always detected in mature B-cells. This sometimes presents as a challenge for clonality determination in clinical flow cytometry. To explore the mechanism and diagnostic significance of slg negative mature B-cells, we retrospectively studied 13 cases of slg negative reactive B-cell lymphocytosis and 88 cases of slg negative mature B-cell lymphomas. The expression patterns of slg and cytoplasmic immunoglobulin (clg) light chain kappa and lambda were studied by flow cytometry using both monoclonal and polyclonal antibodies. These 13 cases of slg negative reactive B-cell lymphocytosis were proven to be polytypic based on cytoplasmic light chain studies. These cases represent the first reported series of body fluids or cystic fluids where reactive B-cells may lose slg, arguing strongly against making a diagnosis of B-cell lymphoma based on lack of slg in mature B-cells. In 88 cases of slg negative mature B-cell lymphomas, we described 4 distinct patterns of abnormal light chain expression including partial or complete loss of slg or clg, suggesting different underlying mechanisms. The findings may help further optimize the light chain evaluation strategy in clinical flow cytometry practice.

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Regional Finalist

Names: Abhinav Ramkumar

High School: Carmel High School, Carmel IN

Mentor: Dr. Horia I. Petrache, Indiana University - Purdue University Indianapolis (IUPUI), Indianapolis, IN

Project Title: Molecular Dynamics of Adenosine Triphosphate Interacting with Phosphatidylcholine Lipid Bilayers.

Adenosine triphosphate (ATP) provides the chemical energy needed in most biological processes from metabolic reactions to cellular mechanics. Hydrolysis of ATP that cleaves phosphate bonds is the mechanism by which energy is released to the environment, resulting in lower energy derivative form of ATP as adenosine diphosphate (ADP) and adenosine monophosphate (AMP). Within biological cells, this chemical reaction often takes place in the vicinity of lipid membranes.

Biophysical experiments by x-ray scattering and NMR spectroscopy have indicated that ATP binds to lipid membranes primarily through the adenine ring, leaving the phosphate chains available for hydrolysis. However, the exact dynamics of ATP, and in particular the possible cooperativity between bound ATP molecules is still unknown. Furthermore, studies suggest the possibility of ATP functioning as a neurotransmitter that works in conjunction with norepinephrine (NE) in sympathetic nerves and is co-released with Acetylcholine (ACh) in parasympathetic nerves and somatic motor neurons; however, knowledge of its chemical and electrical function as a neurotransmitter is incomplete due to the lack of understanding of whether it interacts with membranes and if it is the case, how it does so. This paper examines the interaction of ATP with phosphatidylcholine lipid bilayers to determine its affinity for membranes, which can indicate possible functions as a neurotransmitter.

Molecular Dynamics Simulations reveal that ATP, ADP, and AMP bind to lipid headgroups cooperatively and this behavior generates significant electrostatic charging of membranes even at low concentrations that are typical in biological cells. The important finding is that ATP is directly involved in the electrostatic charging of membranes and this mechanism can affect the transmission of the action potential in neurons.

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Regional Finalist

Names: Pranav Sivakumar

High School: Illinois Mathematics and Science Academy

Mentor: Dr. Donald York

Project Title: Searches for Almost Dark Galaxies in Blank Sky Fields with the Sloan Digital Sky Survey

A class of dwarf galaxies known as Almost Dark Galaxies (ADGs), which are dominated by dark matter and give off little to no starlight, are the ideal laboratories to study the mystery of dark matter. I report results from two distinct approaches developed for detection of ADGs in the Sloan Digital Sky Survey (SDSS). The first approach selects regions called bounding boxes with an uneven light distribution not centered on bright objects. The bounding box approach uses color-cut criteria derived from Leo P, one of the best-known ADGs. This method produced 3,948 targets within SDSS sky coverage; 25 candidates remained following visual review and analysis. The complementary approach targeted ADGs producing absorption lines in quasar spectra by relaxing the Leo P-based color criteria but restricting targets to galaxies with a quasar within 30 arcseconds of the target. The second approach generated 4,516 targets, from which 110 potential candidates were identified based on characteristics of absorption lines of ionized calcium seen in the spectra of background quasars. The most exciting results so far are the confirmations of Leo P and AGC 198691. Plans are underway to obtain narrow-band 21 cm long-integration spectra using the MeerKAT radio telescope to confirm the candidates.

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Regional Finalist

Names: Zoe Solt

High School: Hathaway Brown

Mentor: Dr. Berezovsky

Project Title: Domain wall motion in concave ferromagnetic nanowires

Spin-based electronics require strong, local, rapidly-tunable magnetic fields to affect individual electron spins. Domain walls (DWs) in ferromagnets produce such fields as the magnetization rotates over distances of about tens of nanometers. DWs move relative to energy minima with the application of a magnetic field, and defects in the material known as pinning sites strongly affect their motion. Thus, different geometries facilitate different DW motion. To develop a predictable way of controlling DW motion with a magnetic field for spin-based electronic applications, OOMMF (Object Oriented MicroMagnetic Framework) simulations of different permalloy nanowire geometries were conducted, where DWs were translated with magnetic fields ranging from 1 to 10 mT. A concave structure with a natural energy minimum is the best geometry for predictable DW motion. These simulations yielded constants needed in an analytical model to predict the motion of DWs in concave nanowires with different dimensions. Concave Permalloy nanowires were then fabricated and stable DWs were observed with a sensitive magneto-optical microscopy technique. The pinning of the DWs was investigated, characterizing the DW displacement. It was found that concave nanowires could produce stable DWs that can be moved between pinning sites, creating a mechanism for precise domain wall positioning.

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Regional Finalist

Names: ¹Emily Sun, ²Jessica Mo, ²John Wang

High School: ¹Park Tudor School, ²Carmel High School

Mentor: Tao Lu, Indiana University School of Medicine

Project Title: Using a novel AlphaLISA technique to discover a PRMT5 inhibitor to treat colorectal cancer

Colorectal cancer (CRC) is the second leading cause of cancer related deaths in the United States. Despite important advances in recent years, more than 40% of patients continue to experience disease recurrence following primary therapy. Moreover, there is currently “no cure” for a significant number of patients presenting with metastasis upon diagnosis. An estimated nearly \$14 billion will be spent on CRC care in the United States in 2016, reflecting the urgent medical need for the discovery of novel CRC treatment options. In this study, we identified the protein arginine methyltransferase 5 (PRMT5) as a novel tumor promoter in CRC and successfully developed a highly innovative PRMT5-specific AlphaLISA high throughput (HTS) technique to screen for small molecule inhibitors of PRMT5. Recently, Merck Pharmaceuticals committed \$515 million to screen for the novel inhibitors of PRMT5, testifying to the importance of using PRMT5 as a therapeutic target in cancer. With our innovative approach, we discovered a novel inhibitor, L-CM01, that can effectively inhibit PRMT5 activity in CRC. Furthermore, L-CM01 demonstrated great inhibition for PRMT5-mediated NF- κ B activation and CRC progression in *both in vitro* and *in vivo* CRC models. To conclude, we have successfully developed a powerful PRMT5-specific AlphaLISA HTS technique and discovered L-CM01 as a novel inhibitor of PRMT5 in CRC. Future development of derivatives of L-CM01 may lead to unprecedented therapeutic approaches for CRC treatment..

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Regional Finalist

Names: Sushil Upadhyayula

High School: Illinois Mathematics and Science Academy

Mentor: Dr. Soumya Raychaudhuri

Project Title: Exploring Differential Gene Expression in CD4+ T-Cells to Elucidate Pathways and Subsets Involved in Rheumatoid Arthritis

T cells, which actively participate in immune response by killing pathogens in our body, are essential to understanding immune function. However, T cells normally exist in a dormant state. Thus, in order to understand how they react when activated in the human body, we need to stimulate them. Currently, two options for stimulating T cells include PMA+ Ionomycin (PMAI) and anti-Beads-CD3/CD28 (Beads). While PMAI is a potent, cheap chemical that works by directly attacking the cell, the Beads stimulus is a more natural, expensive alternative. It stimulates the T cell by directly binding to the cell's CD3 and CD28 receptors as would antigens in the human body. We not only found that 76% of the genes are differentially expressed between the two stimuli (the natural Beads stimulus results in more gene expression), but also discovered heterogeneity and the existence of subsets of cells within each stimulus by using single-cell RNA-seq. By studying this heterogeneity using Gene Set Enrichment Analysis (GSEA), we found that the biological pathway for cytokine activation is differentially activated within the Beads stimulus and thereby concluded that it is central in explaining human T-cell heterogeneity. Furthermore, in conjunction with prior research that identified 101 risk genes for Rheumatoid Arthritis, we found that there exist subsets within T cells, where one subset has a higher risk for Rheumatoid Arthritis than the other. Therefore, we discovered that we can potentially identify a patient's risk for Rheumatoid Arthritis by simply stimulating his or her T cells with the anti-Beads CD3/CD28 stimulus and analyzing levels of gene expression.

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Names: Brandon J. Wang and Jennifer Wang

High School: University School and Solon High School

Mentor: Bingcheng Wang

Project Title: Restoration of Ephrin-A1 Expression Negatively Regulates Malignant Behaviors of Prostate Cancer Cells

Prostate cancer (PCa) is the second most common cancer in American men. While most of the newly diagnosed PCa cases are benign, about 3% of them are aggressive and kill the patients within five years. Understanding the mechanisms underlying indolent versus aggressive diseases has important basic and clinical significance. Previous studies have shown that overexpression of EphA2 receptor tyrosine kinase is associated with poor prognosis of PCa. However, the molecular basis remains to be elucidated. Because loss of Ephrin-A1 expression has been linked to tumor-promoting effects of EphA2, we hypothesize that the aberrant regulation of Ephrin-A1 expression may contribute to PCa progression. We report here an inverse correlation between Ephrin-A1 and EphA2 expression in a panel of human PCa cell lines, with increasing EphA2 and decreasing Ephrin-A1 expression as the tumors of origin for the cell lines become more aggressive. Using PC3 cells that lost most Ephrin-A1, we found that restoration of Ephrin-A1 expression caused a dramatic decrease in EphA2 level, and attenuated cell migration and soft agar cell growth. We conclude that loss of Ephrin-A1 drives PCa malignant progression. The discovery also suggests that agents simulating the Ephrin-A1 function can be developed as new therapeutics for metastatic prostate cancer.