

2019 Michigan Undergraduate Research Symposium Sample Abstracts

Use the abstracts and elements below as a guide when preparing your abstract.

- 1) What field are you working in and what's the problem/question your research addresses?
- 2) Why does your approach fit this problem/question?
- 3) What did you do?
- 4) What are your results?
- 5) What are the conclusions and impact from this work?

Development and Characterization of Gold Nanoparticles for Plant Genetic Engineering

Plant genetic engineering is poised to strengthen the agricultural, pharmaceutical, and energy industries in the face of climate change and global population growth. However, traditional biomolecule delivery methods to plants are limited by low efficiency, narrow host range, toxicity, and limited practical applicability due to the transport challenge posed by the plant cell wall. Nanomaterials have highly tunable physicochemical properties that can be harnessed to address these limitations. In this work, we design and characterize gold nanoparticles, tuning key properties such as size, charge, and surface composition to evaluate bio-cargo delivery efficiency into plant cells of mature leaves. In a layer-by-layer self-assembly approach (A), cationic gold nanoparticles (AuNPs) were separately layered with anionic cargo: small interfering RNA (siRNA) or plasmid DNA (pDNA) for gene silencing or expression, respectively. Subsequently, a cationic fusion peptide with a plant cell-penetrating capability served as the terminal layer. In another approach (B), siRNA was directly hybridized to the surface of AuNPs. siRNA constructs from B administered to transgenic GFP-expressing *Nicotiana benthamiana* mature leaves revealed a significant decrease in mRNA levels and a 45% decrease in GFP levels. siRNA constructs from A revealed no significant mRNA silencing but western blot data illustrated a 48% decrease in GFP levels. Additionally, confocal imaging results revealed modest levels of GFP expression in mature leaves of wild-type *Nicotiana benthamiana* with pDNA constructs of A. The systematic investigation of optimal delivery vehicle characteristics in this work provides early insights into the elusive structure-function relationship of nanoparticle transport in plant tissue.

Computational Catalysis: Creating a User-Friendly Tool for Research and Education

Catalysis is used in a significant portion of production processes in the industrialized world, including most processing of chemicals and fuels. This makes maximizing the efficiency of catalysts a high priority. However, the immense number of candidates for new catalysts precludes the possibility of testing all of them by experiments. Density functional theory (DFT) has been widely and successfully used to calculate material properties relevant to catalysis and to screen promising candidates for experimental testing, but there currently exists no publicly-available, user-friendly tool for performing these DFT calculations. This work details the development of such a tool for nanoHUB.org using Quantum Espresso and the Atomic Simulation Environment Python library. Testing was performed for a variety of preloaded structures and surfaces to determine the optimal input values for achieving accurate results in minimal time. The tool's capabilities were evaluated by benchmarking its results against those of previous computational work. The close agreement of these results indicates the readiness of the tool for use in research, and the user interface will enable its use in education to teach students about catalysis and to inspire the next generation of researchers in the field.

Thermodynamic models to aid the experimental design of multivalent systems: Polymer brushes and nanoparticles

Recently, there has been an upsurge in developing pharmaceutical agents with high specificity through multivalent interactions, with nanoparticles being one of the most prominent applications. Multivalent interactions, which involve two different biological entities binding through multiple ligands and receptors, are often seen in nature when a tight bond cannot be achieved with weak univalent protein-ligand interactions. As the ligand binds to the protein receptor, the subsequent intramolecular interactions are much more favorable due to the proximity effect; as such, the overall strength of the multiple affinities increases. However, a nanoparticle can be designed many ways, and as such, a model of the different variations is important in determining which one better suits the criteria. Herein, we explore the binding states of Janus particles—where the different ligands are distributed in patches, and of randomly distributed homogenous particles. We have designed a MATLAB program that is able to determine the percentage of bound species with adaptable parameters, such as ligand density, length, percentage, and nanoparticle design. Additionally, it is able to determine the distribution of the bound states. This program could lead to better design of nanoparticles for increased uptake within the desired cells and more accurate drug delivery.

Temporal changes in *Pseudomonas aeruginosa* flagellar control during early biofilm formation

Biofilms, or aggregate bacterial communities that associate with an interface, exist in nearly every ecological niche and are phenotypically distinct from free-living, planktonic bacteria. The control of cellular motility is key in the bacterial transition from a planktonic lifestyle into the sessile lifestyle necessitated by biofilm formation. While the key regulators of motility during biofilm formation have been identified, little is known about the temporal progression of this process. Recent work in the Wong Lab has demonstrated opportunistic pathogen *Pseudomonas aeruginosa* exhibits a multigenerational “memory” of the surface mediated by second messengers such as cAMP. In this study, we examined whether this multigenerational memory extends to the control of motility. Using a multigenerational single-cell tracking technique, we analyzed the temporal changes in flagellar control in wild-type *P. aeruginosa* and an isogenic PilA mutant lacking functional type-IV pili during early stages of biofilm formation. We found that wild-type daughter cells that inherit the flagella leave the surface at a significantly higher frequency than those that do not. Interestingly, PilA mutant daughter cells with or without flagella leave the surface at about the same frequency. These data suggest that in early stages of biofilm formation, functional pili are required to maintain a specific subpopulation of bacteria at the surface. Cells without functional pili are deficient at maintaining this population, and thus exhibit delayed biofilm formation.

Electrocatalytic Bis(bipyridine)ruthenium Hydroxylation of Tertiary and Benzylic C–H Bonds

The Sigman and Du Bois labs recently reported a methodology that employs a bis(bipyridine)Ru catalyst operating in acidic water to achieve oxidation of tertiary and benzylic C–H bonds in the presence of basic amines. The published method requires a stoichiometric amount of periodic acid to generate and turnover the active catalyst species. Efforts toward the development of an electrocatalytic method for generating the active catalyst in solution are disclosed. Performing the reaction electrocatalytically eliminates the need for periodic acid. Furthermore, the absence of periodic acid opens the possibility for broadening the functional group tolerance as well as reducing the amount of waste generated.