RII Track–2 FEC Emergent Polymer Sensing Technologies for Gulf Coast Water Quality Monitoring

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Gulf of Mexico

The MS Sound and the MS/AL Gulf Coast represent a critical nexus of food-energy-water (FEW) for the region and the greater United States, hosting important fisheries, aquaculture, trading ports, and off-shore oil exploration and production industries. While the exploitation of the region's abundant resources provides critical support to the human population and the economy, the ecosystem is severely taxed by factors including rising CO_2 levels resulting in ocean acidification, agricultural run-off and organic matter thought to be related to hypoxia and "dead zones", and polycyclic aromatic hydrocarbons (PAHs) resulting from oil spills. Assessing and managing sustainable resource utilization in the Gulf Coast will require rapidly deployable, portable, multifunctional, highly sensitive, and specific sensors for the detection of aquatic contaminants.

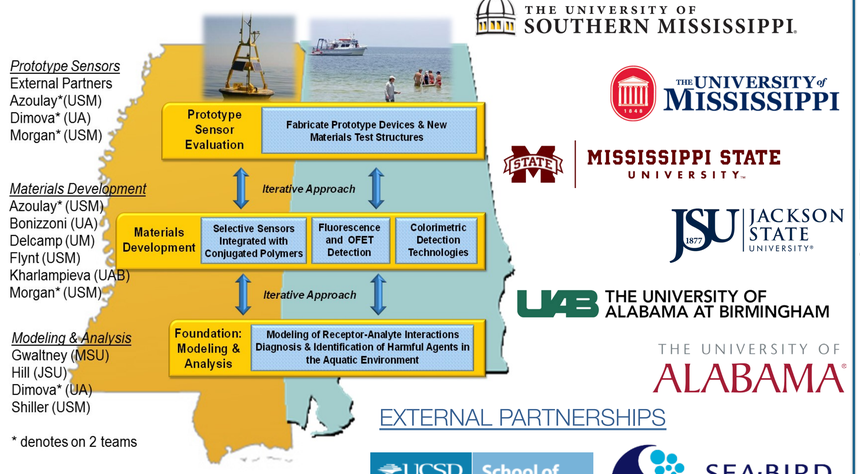
Sensing Platforms

These contaminants (CO_2, nitrates, phosphates, and PAHs) represent a major technological hurdle in the development of robust, rapid, sensing platforms for water quality monitoring - *critical FEW problem*.

"A consortium of Federal Agencies, led by the Presidents Office of Science and Technology Policy has challenged the community to develop simple, robust sensors for Nitrate and Phosphate, as nutrient pollution accounts for one of the nations largest and most complex environmental problems"

Participants / R&D Overview

Interdisciplinary effort bringing together ten researchers with expertise spanning chemistry, biochemistry, geochemistry, marine science, computational science, and polymer science & engineering focused on the goal of the development of portable and rapidly deployable polymer-based sensing technologies for detection of specific analytes.



EXTERNAL PARTNERSHIPS

THE UNIVERSITY OF SOUTHERN MISSISSIPPI · THE UNIVERSITY of MISSISSIPPI · MISSISSIPPI STATE UNIVERSITY · JACKSON STATE UNIVERSITY · THE UNIVERSITY OF ALABAMA AT BIRMINGHAM · THE UNIVERSITY OF ALABAMA · UCSD Jacobs School of Engineering · SEA-BIRD SCIENTIFIC

Research Objectives

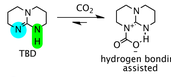
- Develop computational tools to model polymer-receptor-analyte interactions and effectively simulate processes in advanced polymer based sensors
- Design specific receptors for CO_2, nitrates, phosphates, and PAHs for incorporation in organic field effect transistor (OFET), fluorescence, and colorimetric sensing technologies
- Incorporate receptors into polymeric systems and develop broadly applicable analytical techniques for contaminants in Gulf Coast water samples
- Acquire a high precision deposition system and testing equipment for fabrication of devices and characterization of electrical properties for shared use
- Fabricate and test prototype devices and material test structures in collaboration with partners
- Implement "seed grant" competitions for new faculty to increase impact of program
- Sustain research efforts through partnerships with industry, national labs, academic institutions and through collaborative proposal submissions

THRUST 1. Novel Receptors & Polymer Integration

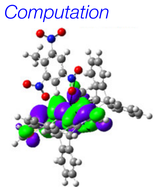
Tasks
Model Analyte-Receptor Interactions
Receptor Synthesis
Binding Studies & Optimization
Monomer & CP Synthesis
Characterization
Fluorescence Modulation
Photophysical Characterization

Products
New Specific Receptor Chemistries
Structure-Function Relationships
Functional Fluorescence Detection
Integration with Thrusts II & III

Receptor Synthesis/Development



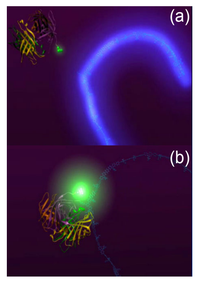
Computation



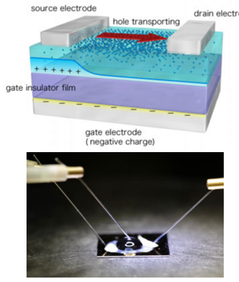
Conjugated Polymer Integration

THRUST 2. Fluorescence & OFET Detection

Fluorescence Assays (Optical)



OFETs (Electrical Transduction)



Tasks
Model Analyte-Receptor-Polymer Interactions
Fluorescence Quenching Assays
FRET Detection of PAHs
Acquisition & Installion of Equipment
OFET Fabrication & Characterization
Evaluation of New Receptor Chemistries
Identification of Water Stable Polymers
Optimization of Polymer-Receptor Devices

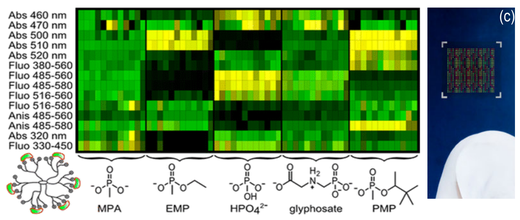
Products
Infrastructure Development
Specific Fluorescence Assays
Specific Electronic Detection
Structure-Function-Property Relationships
Future Research Collaborations & Additional Joint Funding Efforts

THRUST 3. Ensemble Colorimetric Detection

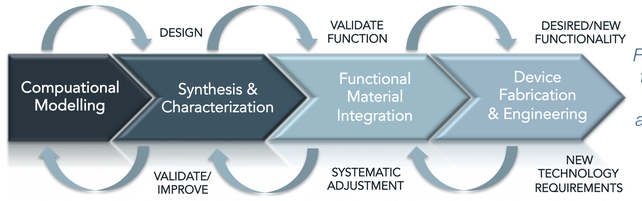
Tasks
Contaminant Characterization & Quantification
Develop Hydrogel Chemistries
Develop Hydrogel Sensing Platforms
Integration of **T1** & **T2** Technologies
Engineering of Optimal Systems
Detector Validation
Multivariate & Statistical Analysis

Products
Advanced Compuational Tools
Optimized Analytical Sensing Systems
New Sensing Paradigms
Improved Analyte Discrimination

Array Based Sensing



T1 + T2 + T3 Integration & Sustainability



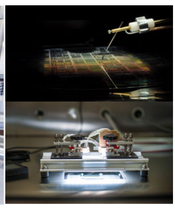
Fundamental nature of the technologies/tools being developed & broad applicability to a variety of sensing technologies

(1) Pursuit of federal funding during and after the project timeline
(2) Evolution of technologies (other analytes, biosensors, engineering: lab on chip, microfluidics, etc.)
(3) Engagement with industrial partners and workforce development
(4) Interdisciplinary research to address the evolving technical complexity of critical FEW challenges
(5) Faculty will be required to submit at least one collaborative publication and one collaborative proposal in years 2–4 of the grant

Infrastructure Development

State-of-the-art device fabrication & testing capabilities

- Unique in states of MS & AL
- Foundational infrastructure
- Support future research collaborations & joint funding efforts
- Sustain research in CPs, sensing technologies, and electronic materials



Workforce Development

Grow the scientific workforce capable of studying and managing FEW systems through education and other professional development opportunities

- Interdisciplinary research, drive collaboration, and focus on junior faculty development
- Professional development workshops including icebreakers, teambuilding, understanding individual communication styles, developing high performance teams & conflict resolution
- Competition for seed grants for junior faculty totaling $50,000
- Graduate student/Post-Doctoral bi-weekly webinars
- Promising technologies will be down-selected in Year 3 for prototype development and testing in the Gulf in Year 4 with SeaBird Scientific

Education & Outreach

- 10 undergraduates will join research teams
- Summer REU program for 10 undergraduates
- 10 high school students from HBCUs and minority-serving institutions will participate in summer or after school research
- Annual events bringing local students to the college campuses.
- Faculty and student visits to local high schools
- Engagement of PSC and CHE students in field work
- Science Cafes

Education day on the RV Point Sur for program participants & student poster session at USMs Gulf Coast Campus

1. Allan, S. E.; Smith, B. W.; Anderson, K. A. *Environ. Sci. Tech.* **2012**, *46*, 2033-2039.
2. McQuade, D. T.; Pullen, A. E.; Swager, T. M. *Chem. Rev.* **2000**, *100*, 2537-2574.
3. Wang, C.; Dong, H.; Hu, W.; Liu, Y.; Zhu, D. *Chem. Rev.* **2012**, *112*, 2208-2267.
4. Liu, Y. L.; Bonizzoni, M. *J. Am. Chem. Soc.* **2014**, *136*, 14223-14229.
5. Knopfmacher, O.; Hammock, M. L.; Appleton, A. L.; Schwartz, G.; Mei, J.; Lei, T.; Pei, J.; Bao, Z. *Nat. Commun.* **2014**, *5*, 2954.