Chemistries for Targeted Delivery of Agrochemicals: Development and Feasibility Testing

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Motivation

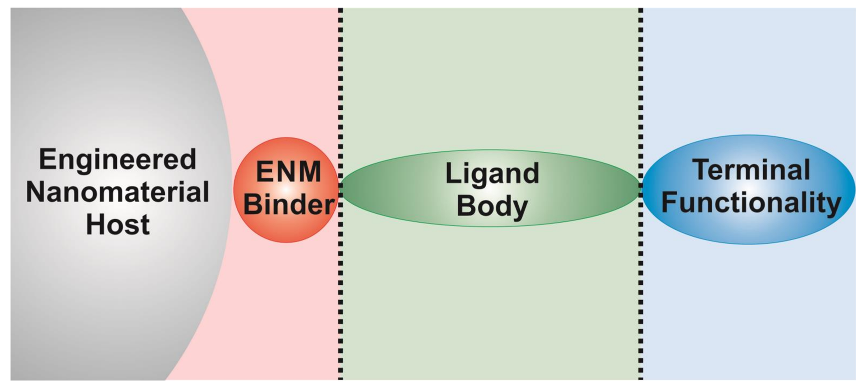
- 187 million metric tons of fertilizer and 4 million tons of pesticides are used globally each year to produce crops.[1,2]
- The average utilization efficiency of N is 50%, P is 20%, and pesticides is 20%.
- The agrochemical fraction that is not taken up by the plant leads to incredible waste and ecosystem degradation, for example:
  - 158 PJ wasted annually based on U.S. ammonia consumption[3]
  - Over 37,000 km^2 of eutrophic waters[4] and persistent pollutants in drinking water sources[5]

Project Description

- My <u>long-term goal</u> is to demonstrate – at field scale – more efficient delivery of agrochemicals to crops through adaptable, targeted agrochemical carriers.
- <u>This seeding grant</u> will be the first step towards pursuing my goal by (i) identifying unique target compounds in/near the root, leaf surface, and internal plant cells, and (ii) demonstrating the preferred interaction of candidate terminal functionalities.

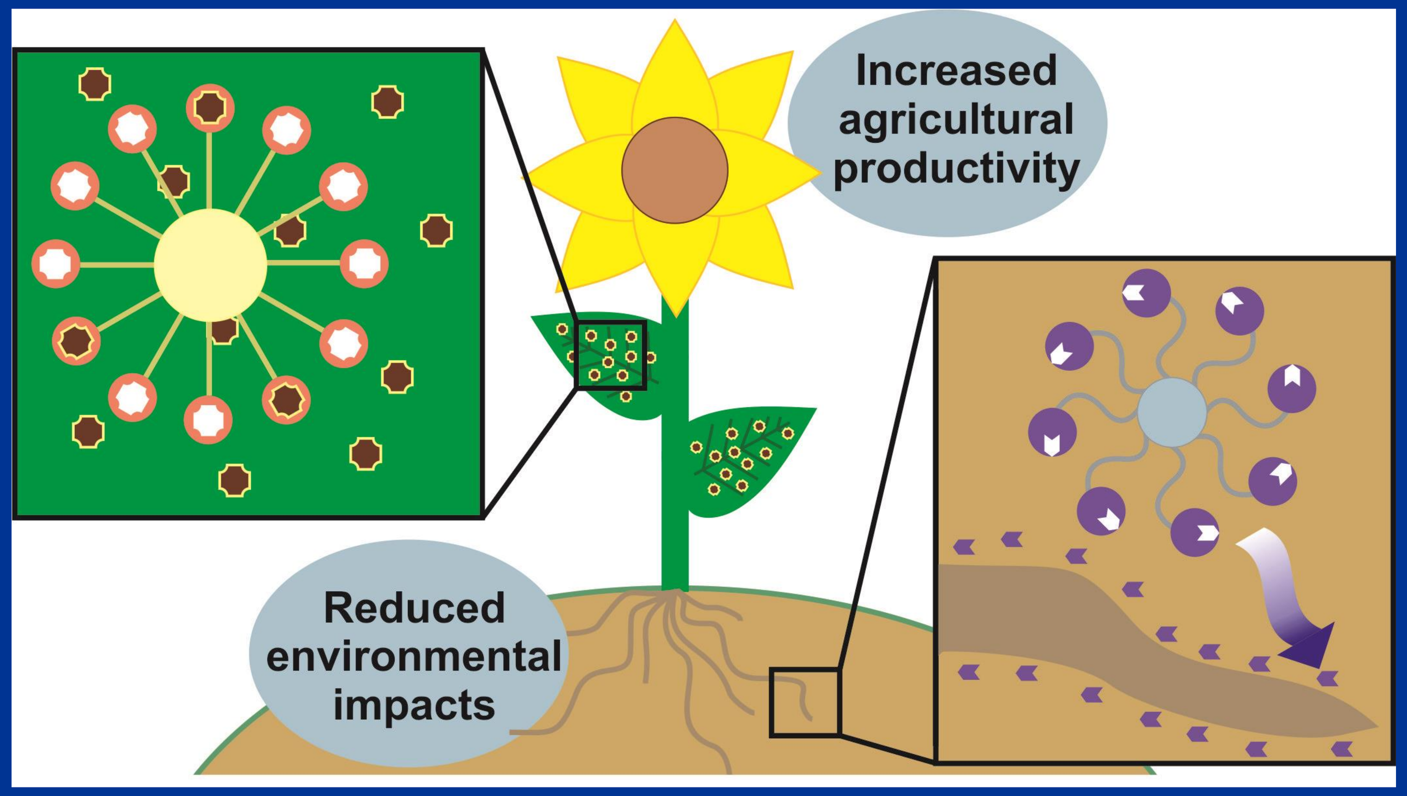
Context

- Best management practices have been around for decades, yet cannot solve this grand challenge
- Nanotechnology is one proposed approach that promises to enhance crop production while reducing agrochemical inputs by leveraging unique properties that emerge from the nano length scale (10^{-9} m)[6,7,8]
- I propose that additional opportunities exist in the design and development of terminal surface chemistries that can target specific components of the crop.



University of Pittsburgh

Advance sustainable agriculture and rebalance critical nutrient cycles through the development of chemistries that target the delivery of agrochemicals to plants.

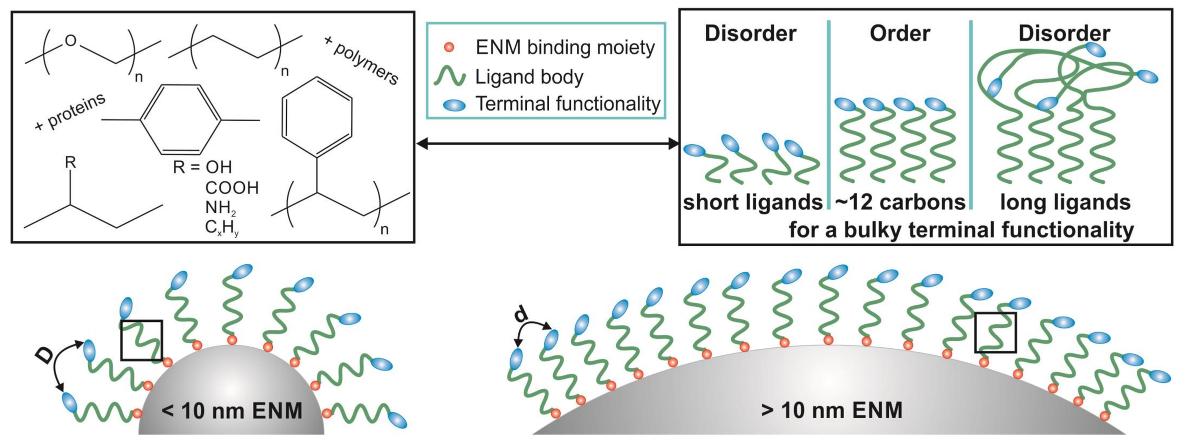


Project Deliverables

- At the end of the 1-year funding period, we will have identified targets and targeting chemistries (expanding the following table[9]) as well as demonstrated their binding affinity through existing and novel assays.

Location	Target compound	Targeting moiety	Type of interaction	Active ingredient class of interest
Rhizosphere	Glucose	Lectin from pea[38], Synthetic lectin[39]	CH-π and polar interactions	Fertilizers
Rhizosphere (under stress)	Flavonoids	Bovine serum albumin (BSA)[40]	Protein-ligand interaction	Fertilizers
Leaf	1° and 2 ° alcohols	Poly-l-proline (homopolymer)[41]	H-bonding	Pesticides
Leaf with Karnal bunt	Phenols	Bovine serum albumin (BSA)[42]	Protein-ligand interaction	Fungicides (e.g., propiconozol or mancozeb)
	Trimethylamine	Casein[43]		

- Results from this seed project will lay the foundation for future work to develop the platforms – connecting the identified terminal chemistries to an agrochemical carrier (e.g., below[9]) – and demonstration of success in plant systems.



Potential Impact

- Crop production has a massive impact on our environment and global well being. It also suffers from extreme inefficiencies that can be addressed with innovative approaches to re-balancing critical resource cycles.
- If successful, this work has the potential to preserve finite resources, reestablish aquatic ecosystems and the economies and communities that depend on them, and protect drinking water sources; collectively advancing agriculture, sustainably.

References and Acknowledgements

- [1] Zhang, W. *PNAS* 2018, 8(1), 1-27 [2] Food and Agriculture Organization of the United Nations. *World Fertilizer Trends and Outlook 2020*, 2017 [3] USDA ERS. Fertilizer Use and Prices database [4] Rabalais, N. N.; et al. *ICES J. Mar. Sci.* 2009, 66(7), 1528-1537. [5] Klarich, K. L.; et al. *ES&T Lett.* 2017, 4(5), 168-173 [6] Kah, M.; et al. *Nat. Nanotechnol.* 2019, 14(6), 532. [7] Giraldo, J. P.; et al. *Nat. Nanotechnol.* 2019, 14(6), 541 [8]Lowry, G.V.; Gilbertson, L. M.; et al. *Nat. Nanotechnol.* 2019, 14(6), 517. [9] Smith, A. M. and Gilbertson, L. M. *ACS Sus. Chem. Eng.* 2018, 6, 13599

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