Sustainable Hydrogels for Water Treatment

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A major challenge in water treatment today is the elimination of micropollutants, including low-concentration emerging contaminants like PFAS and heavy metals like lead. Existing technologies like activated carbon adsorption fail to eliminate these contaminants due to their chemical diversity and low concentrations (micrograms to nanograms per liter). Yet, it is important to be able to remove micropollutants from water to promote human health, comply with increasingly stringent laws and regulations, and enable technological development. Given that wastewater treatment is responsible for 5% of global greenhouse gas emissions, the space limitations on the sizes of treatment processes (such as in large cities), and resource constraints (in developing markets, which suffer from the greatest water pressure), it is also important to develop methods to eliminate micropollutants sustainably, and in low-footprint, resource-efficient processes.

Hydrogels (polymer gels containing a significant quantity of bound water) are an ideal platform for the development of new functional materials to bind and degrade micropollutants. Water-based chemistry and a large library of commoditized precursors allow significant chemical flexibility to design for desired performance. High porosity and water content allow rapid transport of micropollutants, reducing equipment footprint and operating costs. A principal theme in this thesis is the unified design of hydrogel materials at multiple length scales using a combination of theory, simulations, and experiments - from chemistry control to engineering scale up. Special emphasis is laid on filling market niches and addressing real-world problems by means of practical solutions throughout the technology development process.

First, we focus on technologies to sequester micropollutants using hydrogel absorbents. Using rational design principles that combine simulations and experiments, we synthesize hydrogels bearing multiple functionalities, including chemically anchored micelles to bind organic micropollutants, and chelating agents and charged groups to bind metal cations. Hydrogel microparticle absorbents are shown to treat complex contaminated water at environmentally relevant concentrations, including in the presence of background hardness. A proof-of-concept packed bed demonstrates the scalability of this approach. In an academia-industry collaboration, these hydrogel microparticles are tuned to treat amino acid fermentation products, selectively removing impurities without eliminating the target amino acid. The hydrogels achieve performance comparable to commercial adsorbents, while simultaneously being more sustainable and versatile. We also further develop hydrogels as a platform technology for sequestration applications, preparing hydrogel capsules to hold yeast cells for water treatment, aiding in the scalability of biological treatment methods by eliminating the need for secondary steps to remove added microorganisms from water.

Next, we present a solution to degrade organic micropollutants, based on binding single-atom iron inside hydrogel microparticles. Iron is used to catalyze a Fenton reaction, converting added hydrogen peroxide to highly reactive hydroxyl radicals that oxidize hazardous organic micropollutants into safer small molecules. An appropriate chemistry allows us to implement the Fenton reaction, which normally requires an acidic environment, loses catalyst in the form of sludge, is footprint-intensive, and suited to the destruction of relatively high concentration contaminant streams, without suffering from these traditional limitations. We demonstrate the degradation of recalcitrant micropollutants, providing a pathway to their accelerated elimination from the environment.

Finally, we turn to the scale up and application of this technology in real-world settings. Highlighting evolving regulations and improvements in our understanding of water quality, we present a series of case studies focusing on industrial applications such as food & beverage and semiconductor manufacturing, and oil and gas extraction. Of special importance here are the diverse practical considerations and market constraints that must be overcome to promote technology adoption. Within this context, we discuss how technologies like those introduced in this thesis could enable versatile and low-cost effluent treatment for regulatory compliance, and tunable and selective treatment of influents and process streams to enable high-quality manufacturing. We present a method for scaling up the manufacturing of our hydrogel materials, and discuss some recent steps taken towards the commercialization of this technology.

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