Center for Bio-Inspired Energy Science (CBES)
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Lead Institution: Northwestern University
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Mission Statement*: To develop the next frontier in soft materials relevant to energy challenges by designing structures that emulate functions we see in biological systems.*

Soft materials are normally composed fully or partially of organic matter and the best examples are polymers, which have had an enormous impact in energy relevant technologies, particularly energy savings in transportation, manufacturing, infrastructure, and construction, among others. The next challenge is to learn how to synthesize soft materials with the capacity to interconvert energy forms, for example the way muscles convert chemical to mechanical energy in living organisms, or the way plant leaves optimize conversion of light to chemical energy. Our proposed research program specifically tackles the next big challenges in synthetic design of soft materials, namely learning how to molecularly encode in them the ability to transduce energy and even move autonomously in ways that are characteristic of "living matter". We approach this enormous bio-inspired challenge through bottom–up chemical design and synthesis combined with top–down engineering strategies, computation, and theory to create novel functional systems. The goal is to develop new opportunities around the concept of "robotic soft matter", denoting its autonomous ability to rapidly perform mechanical, optical, or chemical tasks with only small inputs of energy and without the use of complex hardware. Equally important is learning to create "photosynthetic matter", which requires systems structured holistically to enable efficient chemical production using visible light. Our targets to create robotic and photosynthetic soft matter are extremely relevant to future modalities in manufacturing and chemical production. Our cross-disciplinary investigations focus on bio-inspired research in the following areas.

Task 1: "Multi-Scale Synthesis of Artificial Muscles"
Building on computational and experimental design of light-responsive hydrogel walkers and photoresponsive heterogeneous origami gels developed in CBES during the last funding cycle, we will explore new light-responsive hydrogels containing supramolecular polymers that undergo more complex responsive motion, such as swimming toward a light source. Our continuum models are being used to describe the swimming mechanism and the possible origin of phototactic behavior. We will continue to optimize the performance of the swimmer and we will perform simulations for different conformations and robot designs capable of performing various shape transformations for targeted functions. The modeling will include the development of time-dependent, light-responsive hydrogel models that will incorporate multiple reversible transformation mechanisms for robots.

Task 2: "Magnetic Morphogenesis"
CBES researchers have studied the equation of state that arises in a system of colloidal rotors driven by a magnetic field on an inclined surface, which shows unusual behavior with changes in viscosity and frequency of rotation. It has become apparent that we need to include hydrodynamic codes developed by CBES to understand the phenomenon. For example, we are now considering "odd viscosity", which arises if time reversal is broken, in Stokesian dynamics of bulk systems.

Task 3: "Autonomous Soft Microrobots"
During the last funding period, CBES developed Quincke oscillators obtained from micron-scale colloids in a static electric based on the charging and actuation of particles within a field-induced boundary layer. The Quincke oscillation mechanism provides a useful experimental model for active matter composed of

many self-oscillating units where particle interactions depend on oscillator orientation and phase to mediate their collective dynamics. Experiments on ensembles of Quincke oscillators have recently revealed new emergent assemblies such as oscillating vortex crystals, where oscillators synchronize and orient within close-packed lattices. We are developing a dynamic model of multiple Quincke oscillations to understand the synchronization and alignment of two oscillators mediated by electrostatic and hydrodynamic interactions. We have also developed active colloids and other soft-matter systems that exhibit internal control mechanisms for achieving autonomous functions like gradient-driven navigation. We are developing a highly dynamic coacervate system based on enzymes in a chemostatted chamber to enable the experimental study of liquid droplets with internal feedback mechanisms based on chemical fuels. In this system, the chemostatted environment promotes drop formation, while the enzymatic reaction within the droplet promotes its dissolution to create dynamic droplets of a prescribed size.

Task 4 "Hierarchical Structure-Mediated Photocatalysis"

As part of our previous studies on non-equilibrium phenomena in hydrogels, we discovered colloidal crystal metallization in binary crystals of size-asymmetric DNA-functionalized nanoparticles with complementary end nucleotide sequences. At the metallization transition, the small component lattice melts. We are now analyzing the dynamic behavior of size-asymmetric charged colloidal particles under an external electric field when the large nanoparticles are connected by polymeric springs. Preliminary work suggests a dynamic transition to a state where the small particles condense into clusters under high electric fields. This work will demonstrate a new way of transporting charge that will be useful for the design of devices with controlled transport, including batteries.

Task 5: "Mechanical Enhancement of Photocatalysis"

Movement in photosynthetic organisms regulates a series of processes that are necessary to maximize light absorption, control gas exchange, and regulate water loss, among other functions. We recently discovered a novel self-assembled system that photocatalytically produces hydrogen peroxide without the need for a metal catalyst. By integrating this supramolecular polymer into a thermoresponsive polymer scaffold, we found that the photocatalytic reaction rates can be controlled by changing temperature. With heating and cooling cycles, the photocatalysis rate increases with the actuation rates due to enhanced flow of water and solutes in and out of the hydrogel. The demonstration that actuation can regulate and even enhance the photocatalytic rates provides a framework for designing future lifelike artificial photosynthetic systems.

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