

and exceptional biocompatibility should prove valuable for bionanofluidic and cellular interface applications.

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Titration Properties and pH-Dependent Aggregation of Chitosan

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Chitosan is a polysaccharide consisting of N-acetyl-glucosamine and glucosamine units, prepared by the deacetylation of chitin. Glucosamine contains an ionizable primary amine, rendering chitosan water-soluble at low pH and insoluble at pH above ~6.5. This pH dependent solubility can be exploited to make hydrogels used for coatings and sensors. We have used constant-pH molecular dynamics (CpHMD) to investigate the pH dependence of chitosan. Starting from a stable aggregate of neutral chitosan, we performed replica exchange simulations over a pH range 4.0-8.5. The aggregate remains stable at high pH and dissociates at low pH, as expected. Interestingly, the transition occurs cooperatively at around pH 6.5, in a remarkable agreement with experiment. The calculated bulk pKa was found to be similar to the transition pH, again in agreement with experiment. The role of electrostatic interactions and aggregation-induced desolvation in the protonation equilibria of the amine groups was also examined. This work provides atomic-level insight into the pH-dependent behavior of chitosan which may aid in the design and development of various chitosan-based materials.

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Using Spores of *Bacillus* to Create Evaporation-Driven Engines

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Biological organisms harness energy from natural evaporation by using their inherent structures which are able to capture and stretch water molecules in response to the chemical potential gradient of water. A tree is a simple example, where water is continuously transported to the top, sometimes one hundred meters above the ground, due to evaporation occurring at the leaves. These stimuli-responsive biomaterials could possibly exhibit high energy densities for efficient energy converters and actuators. *Bacillus* spore is a water-responsive biomaterial that has a large energy density, high reversibility, and fast response to variations in relative humidity (RH). Here, we present hybrid spore/plastic biomaterials that can be used for high strain actuation and energy harvesting from evaporation. We fabricated the spore/plastic hybrid biomaterials by periodically coating alternating sides of ultrathin polyimide tapes with bacterial spores. The resulting structure curved into an approximately sinusoidal shape with a low RH nearby, and achieved a large linear displacement at both ends of the tape. By exchanging less than 5% water by weight, these hybrid biomaterials produced a large actuation strain of ~200 % and a fast response (< 1s) due to changes of RH. The actuation displacement and force can be easily scaled up by assembling these hybrid biomaterials in series and parallel. Using these packaged hybrid biomaterials, we created two types of evaporation-driven engines that convert evaporation energy to oscillatory and rotary motion. When we placed these engines near wet surfaces, they start and run autonomously and produce work continuously. We demonstrated that the mechanical work is sufficient to power a light source and drive a miniature car.

References:

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2464-Pos Board B601

Transport Properties of Carbon Nanotube Porins in Lipid Vesicles

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Cells differ in their individual permeabilities depending on what lipids and proteins are present in the membrane and by regulating the number of channel

proteins present in their system. The maintenance and regulation of ion gradients, specifically the electrochemical proton gradient, $\Delta\mu\text{H}^+$, across biological membranes has been established as a necessary intermediate in biological energy transduction that is crucial for proper cellular function. In recent years, artificial membrane channels have attracted much attention due to the key role of proton channels in performing a number of specific functions in different cells. Carbon nanotube (CNT) structures are similar to biological channels (e.g. aquaporins) with their smooth, narrow (ca. 1.5 nm), hydrophobic inner pores. The hydrophobic walls of the CNT facilitate the formation of 1D hydrogen bonded water chains and results in weak interactions with water molecules that enable nearly frictionless water transport. CNTs can provide a functional mimic of biological channels, and to that end we have created shortened CNT porins and investigated osmotically-driven transport of protons, ions and uncharged species through these pores. This presentation will discuss measurements of transport efficiency and transport selectivity in these biomimetic membrane channels and compare them with properties of biological ion channels.

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Field Effect Transistors Based on Semiconductive Microbially Synthesized Chalcogenide Nanofibers

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Microbial redox activity offers a potentially transformative approach to the low-temperature synthesis of nanostructured inorganic materials. Diverse strains of the dissimilatory metal-reducing bacteria *Shewanella* are known to produce photoactive filamentous arsenic sulfide nanomaterials by reducing arsenate and thiosulfate in anaerobic culture conditions. We present *in situ* microscopic observations and measure the thermally activated (79 kJ/mol) precipitation kinetics of high yield (504 mg per liter of culture, 82% of theoretical maximum) extracellular As_2S_3 nanofibers produced by *Shewanella* sp. strain ANA-3, and demonstrate their potential in functional devices by constructing field effect transistors (FETs) based on individual nanofibers and photoelectrochemical cells based on macroscopic mats. The use of strain ANA-3, which possesses both respiratory and detoxification arsenic reductases, result in significantly faster nanofiber synthesis than other strains previously tested, mutants of ANA-3 deficient in arsenic reduction, and when compared to abiotic arsenic sulfide precipitation from As(III) and S^{2-} . Detailed characterization by electron microscopy, energy-dispersive X-ray spectroscopy, electron probe micro-analysis, and Tauc analysis of UV-Vis spectrophotometry show the biogenic precipitate to consist primarily of amorphous As_2S_3 nanofibers with an indirect optical band gap of 2.37 eV. X-ray diffraction also reveal the presence of crystalline $\text{As}_8\text{S}_{9-x}$ minerals that, until recently, were thought to form only at higher temperatures and hydrothermal conditions. The nanoscale FETs enable a detailed characterization of the charge mobility ($\sim 10^{-5}$ cm²/V s) and gating behavior of the heterogeneously doped nanofibers. We also present a characterization of detected photocurrent. These studies indicate that the biotransformation of metalloids and chalcogens by bacteria enables fast, efficient, sustainable synthesis of technologically relevant chalcogenides for potential electronic and optoelectronic applications.

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Nanomechanical Deformation Behavior of Amyloid Fibrils

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Amyloid fibrils playing a role in disease expression have recently been found to exhibit excellent mechanical properties, which are highly correlated with the biological functions of amyloid fibrils. It has not yet fully understood how amyloid fibrils formed by aggregation of mechanically weak protein chains can exhibit remarkable mechanical properties. In this work, we study the nanomechanical deformation behavior of amyloid fibrils using steered molecular dynamics simulations. It is shown that the length scale of amyloid fibrils is a key factor in determining the nanomechanical deformation mechanisms of amyloid fibrils and their resulting nanomechanical properties. It is attributed to the competition between shear and bending deformations, which depends on the length scale of amyloid fibrils. The length-dependent elastic property of amyloid fibrils has been elucidated based on Timoshenko beam model. Our study sheds light on the importance of the length scale of amyloid fibrils for understanding their nanomechanical properties.