Brief description

Over the last 3.6 billion years, nature has developed processes and materials with exquisite selectivity, specificity, and adaptability. Self-assembly has been one of the many strategies nature uses for generating nanostructures with precise organization, shape and functionalities. Self-assembling proteins are valuable building blocks allowing the construction of materials with versatile chemical properties and functions based on their tertiary and quaternary protein structures. Well-studied motifs from tandem repeat proteins (such as silk, elastin, collagen, keratin, resilin, and squid ring teeth-SRT) have been frequently used to create multifunctional materials for diverse applications exhibiting extraordinary physical responses that have not been observed in materials synthesized via usual routes. Besides their extraction from natural sources, derivatives of these biopolymers are engineered, e.g. via directed evolution. In this networking event, we will discuss in-vitro and in-vivo self-assembly of cellulosics and will address how the structure of the helicoidal order of cellulosic building blocks reflect into their function and material properties. We then focus on using directed evolution to self-assemble tandem repeat biopolymers that can be tuned for predefined macroscopic symmetries, by controlling their packing symmetry or order. State-of-the art experimental and computational tools to predict performance of such genetically engineered materials will be presented and future directions, particularly for utilizing the dynamical properties of these materials, will be discussed.

Format & schedule

Two main speakers; five short talks from selected abstracts; panel discussion and networking time in break-out rooms. Networking event organized by graduate student (Erhan Ekmen – Sabanci U)

16:00-16:10 Opening Remarks (Ali Rana Atilgan – Sabanci U)
16:10-16:50 Ahu Gumrah Dumanli-Parry (U Manchester) – Helicoids and Self-assembly of Polysaccharides
16:50-17:30 Melik Cumhur Demirel (PennState) – Genetic Engineering of Programmable Materials
17:30-17:40 Break
17:40-18:30 Short presentations
  • Kerim Dansuk (Northwestern U) – Simple mechanical models for synthetic catch bonds
  • Aled Roberts (U Manchester) – Non-covalent protein-based adhesives: synthetic spider silk vs. bovine serum albumin
  • Osman Burak Okan (Sisecam Sci.&Tech.) – The prospect of using semiconductor thin films as microbial surfaces on silicate glasses
  • Oguzhan Oguz (EPFL) – Hierarchical self-assembly of damage tolerant polyurethane-urea copolymers resembling spider silk proteins
  • Baris Emre Kiral (Sabanci U) – Predicting In-Plane Uniaxial Compressive Moduli of Hexagonal Honeycombs Using Experimental Analogues
18:30-18:50 Panel discussion – moderator: Ali Rana Atilgan (Sabanci U)
18:55- Zoom break-out rooms open for additional networking
Room SYNTH: Synthetic materials mimicking nature (host: AGD)
Room NATUR: Materials derived from nature (host: MCD)
Room MODEL: Modelling hierarchical materials (host: ARA)
Abstracts

Main speakers

Ahu Gumrah Dumanli-Parry: Helicoids and Self-assembly of Polysaccharides

Over the last 3.6 billion years, nature has developed processes and materials with exquisite selectivity, specificity, and adaptability. Self-assembly has been one of the many strategies nature uses for generating nanostructures with precise organization, shape and functionalities. Cellulose is the most abundant biopolymer on earth. Despite of its commonality and importance in nutritional, agricultural, and industrial production, surprisingly little is known about the genes and enzymes that carry out the synthesis and organisation of their structural fibres in the cell wall. In the most basic form when cellulose polymer chains are secreted inside or outside of cells, they form fibrous structures via weak bonds in an organized way. This adds strength to the entire structure. A recurring structure that can be seen in cellulose, chitin and collagens is the helicoidal structure (like the cholesteric mesophases), i.e. a multi-layer structure where adjacent layers rotate along a helical screw. Such helicoidal formation of fundamental structural fibres play an important role in biology because the combination of order and mobility is a basic requirement for self-organisation and structure formation in living systems. While formation of the liquid crystalline-like self-assembly has key consequences in living matter, they are not fully defined or understood. However, their effect on maximisation of packing efficiency, mechanical performance and optical signature are well known and have been explored.

In this discussion, we will present nature’s cellulosic building blocks at the cell wall. Further, we will discuss their presentation into helicoidal orders that deviate from the monotonic cholesteric structures with graded pitch and random pitch patterns which is always left-handed in terms of optical chirality. Such behaviour provides these structures the propensity to generate complex optical responses. The discussion session will compare the in-vitro and in-vivo self-assembly of celluloses and will address how the structure of the cellulosic building blocks; i.e. their crystallinity, their interactions with hemicelluloses, lignins and microtubules, influence the functional properties in the cell wall.

Melik Cumhur Demirel: Genetic Engineering of Programmable Materials

Self-assembling proteins are valuable building blocks allowing the construction of materials with versatile chemical properties and functions based on their tertiary and quaternary protein structures. Well-studied motifs from tandem repeat proteins (such as silk, elastin, collagen, keratin, resilin, and squid ring teeth-SRT) have been frequently used in combination to create multifunctional materials for diverse applications. Besides their extraction from natural sources, these biopolymers are produced using genetically modified organisms. Over the four billion years of evolution, living organisms produce a variety of biopolymers for specific metabolic functions, mechanical supports or sensing environment. Such materials and their engineered derivatives via directed evolution can exhibit extraordinary physical responses that have not been observed in synthetic or inorganic materials. Those properties and responses selected via directed evolution can play significant roles in achieving novel functionalities and fabricating various devices. Recently, we discovered that tandem repeat biopolymers can be tuned for predefined macroscopic symmetries, which cannot be obtained in traditional materials engineering, by controlling their packing symmetry or order during assembly via directed evolution. Our goal is to create self-assembling materials with unprecedented control over their physical properties using synthetic biology. Moreover, exquisite knowledge of structure-property relationships in proteins will aid in the design of composites materials (organic/inorganic) with desired properties for building devices with novel functionalities, which are difficult to achieve or previously unattainable. For example, we created functional programmable materials with user defined physical properties from composites of 2D-layered materials and polymeric proteins that can break the rules of mixtures for composites materials with properties engineered precisely to optimize superior performance compared to conventional composites. Our approach for composite materials is based on directed evolution to screen molecular morphology of polymeric proteins against 2D-layered materials. The composites can be designed to exhibit a variety of unusual physical properties (e.g., ultra-high thermal storage at room temperature, or thermal conductivity switch, as well as self-healing soft-robotics). In this talk, we will discuss (i) sequence-structure-property relationships for tandem repeat proteins that can be genetically engineered, (ii) self-assembly of hierarchical organic/inorganic structures that can provide dynamic and time-responsive materials, and (iii) experimental and computational tools to predict performance of genetically engineered materials.
Short Talks:

Simple mechanical models for synthetic catch bonds
Kerim Dansuk, Sinan Keten

Catch bonds are protein-ligand bonds which become more difficult to break as the applied force increases, a counterintuitive phenomenon that has not yet been reproduced in synthetic systems. Most designs proposed so far rely on macromolecular linkers with complicated folds rather than particles exhibiting simple dynamic shapes. In this work, we have demonstrated that simple mechanical designs can exhibit catch bond characteristics under thermal excitations. These systems have force-sensitive switches which control the transition of the system to a stronger binding state with the targeted surface either by facilitating secondary interactions or by redistributing the force on acting on the binding members. We performed molecular dynamics simulations to show our designs have force-enhanced bond lifetimes reminiscent of catch bonds. The design concepts presented here for synthetic catch bonds illuminates a path towards novel nanoparticle or colloidal assemblies that have the passive ability to tune the strength of their interfaces with applied force, setting the stage for self-assembling materials with novel mechanical functions and rheological properties.

Non-covalent protein-based adhesives: synthetic spider silk vs. bovine serum albumin
Aled D. Roberts, William Finnigan, Paul P. Kelly, Matthew Faulkner, Rainer Breitling, Eriko Takano, Nigel S. Scrutton, Jonny J. Blaker and Sam Hay

Protein-based adhesives could have several advantages over petroleum-derived alternatives, including lower toxicity and smaller environmental footprint. Here, we demonstrate that non-covalently crosslinked bovine serum albumin (BSA) and recombinant spider silk proteins have high adhesive strength on glass and other transparent substrates. The mechanism of adhesion was primarily attributed to the supramolecular association of β-sheets into a densely hydrogen-bonded network.

The prospect of using semiconductor thin films as microbial surfaces on silicate glasses
Osman Burak Okan, Refika Budakoğlu, Çağdaş Kadakal, Anıl Özen, Gizem Aydın, Zeynep Aydın, Fulya Elgin, Burcu Öğüt

Pristine glass surface is largely inert against microorganisms. Bacteria and viruses can survive for long durations on glass surfaces. For the case of SARS-CoV-2 virus, which is linked with the ongoing COVID-19 pandemic, reported residence time is on the order of days [1]. Ion exchange, most notably with Ag+ ions, has been known endow silicate glasses with antimicrobial properties [2, 3]. Despite being scalable, this procedure is slow and costly, generally cause discoloration, and the biocidal activity of ion exchanged glass entails the leaching of active agents. Suitably chosen antimicrobial thin film coatings based on sub-micron thick oxide semiconductors offer compelling alternatives as they permanently modify the surface electronic structure and enable higher roughness characteristics. Additionally, oxides are known to be more amenable to bacterial adhesion in comparison to uncoated glasses [4]. With this route, the antimicrobial activity with contact killing can be attained without leaching of the active ingredients. Additional requirements such as low visible reflection, low optical haze and non-iridescent appearance can be accommodated with thickness control and the introduction of additional layers. In this talk, we will present the recent progress on the antimicrobial properties of transition metal doped oxide semiconductor thin films deposited with atmospheric pressure chemical vapor deposition (APCVD) techniques. This deposition method is well established for large area coating applications [5]. Depending on the reactor geometry APCVD technique can be used to coat complex shaped articles as it can handle high production line speeds and temperature gradients observed on the glass surface. We will discuss the coated glass performance characteristics in reference to antimicrobial test protocols, possible sources of antibacterial activity, thin film optical properties and demanding mechanical/chemical durability requirements of the industry.

Hierarchical self-assembly of damage tolerant polyurethane-urea copolymers resembling spider silk proteins

Oguzhan Oguz, Nicolas Candau, Eren Simsek, Gregory Stochlet, Cagla Kosak Soz, Ozge Heinz, Emel Yilgor, Iskender Yilgor, Yusuf Z. Menceloglu

The notion of replicating the hierarchical self-assembly of spider silk proteins is of significance for designing synthetic materials with unique combinations of stiffness, strength, extensibility and toughness. However, this is a challenge. In this talk, I will provide an overview on the hierarchical self-assembly of stimuli-responsive polyurethane-urea copolymers identical to that of spider silk proteins. Unlike conventional “silk-inspired” polymers, these materials demonstrate seven levels of structural hierarchy that comprises a replica of each structural element (antiparallel beta-sheet nanocrystals, beta-turns, helices, tertiary network domains, fibrils, fibers) found in silk hierarchy. Just as in silk; (i) the structure formation is driven by geometric confinement, and (ii) the cooperativity of hierarchically organized building blocks ensures unprecedented combinations of stiffness, strength, extensibility and toughness, which can be further reversibly tailored by heat and/or water (hydration) thanks to the stimuli-responsive nature of these copolymers. Our findings reveal how to mimic the silk hierarchy even without using amino acids, but only with a limited set of synthetic basic building blocks. Hence, it may be of interest for various applications.

Predicting In-Plane Uniaxial Compressive Moduli of Hexagonal Honeycombs Using Experimental Analogue

Baris Emre Kiral, Melih Papila

Cellular solids have been utilized in many engineering applications for thermal insulation, their high specific out-of-plane compressive strengths and stiffnesses, their sieving capabilities, and in-plane energy absorption properties. With the advances in additive manufacturing, numerous novel 2D cellular solid designs have emerged. In-plane properties of 2D cellular solids have attracted attention for their intriguing behavior under compressive, tensional and shear loads. As structures deviate from common geometries such as square, triangular, or hexagonal, analytical and numerical methods to predict effective elastic properties get dramatically more convoluted. Thus, analytical models in particular have been limited to the simpler designs. Moreover, validating and/or characterizing experimental analyses of novel geometries are often limited in scope due to size effects and inconsistent constraints among the test specimens and practical structures. This study presents a new approach that amalgamates virtual and real-life static analysis of cellular structures of repeating cells. Representative equivalent structures for testing, i.e. analogue test specimens are determined using parametric FEM analysis. Analogues for hexagonal honeycomb arrays are manufactured and tested under compression. Compressive moduli of the selected analogues exhibit great consistency between numerical and experimental analyses. The approach sets a framework for future research in using analogues for determination of in-plane properties of numerous other 2D cellular solid designs.