reconstituted as near-native membrane proteins within artificial bilayer systems could be utilized in formulating bioactive surfaces for powerful biomedical and biosensor applications. Novel techniques for re-forming the full-length IMP construct will be discussed.

3190-Pos Board B620

Characterization of Peptides Designed to Control Crystal Nucleation and Growth

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Organisms, from algae to humans are known to mold complex, hierarchical hard tissues from minerals using biomolecular templates and additives. Molecular-level mechanistic understanding of how these biomolecules, particularly proteins, participate in the nucleation and growth of these inorganic crystals has been a longstanding goal. We design peptides with transformative abilities over calcite crystals using Rosetta. Based on the theory of how additives alter crystal nucleation and growth, we employ four modification strategies to modify the morphology of the crystal, viz. a peptide binding to a face, an array of peptides binding to a face, peptides pinning steps and peptides blocking kinks. To test the designs, we employ a variety of techniques ranging from measurements at the atomic scale to full crystal observations. We also investigate alternative mechanisms of modification by comparing the interactions predicted by Rosetta in other select states to those in the target state. For each design, we obtain the solution-state structure of the peptide by circular dichroism. To test peptides designed against a non-native face of calcite, we artificially stabilize the face for binding measurements. The overall crystal morphology change is then tested by incubating supersaturated precursor solutions with the design peptides. To confirm the predicted mechanism of growth alternation, we observe the change in kinetics of calcite step growth with peptide doping using in situ AFM, and report calcite step velocities. Finally, by nucleating calcite on a monolayer of the designed peptides, we examine the face on which calcite nucleated and compare it to our target face. These experimental results provide a feedback loop to the next generation of designs and enable the rational design of bio-surface interactions.

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Examining Bacterial Cell Interactions using Atomic Force Microscopy

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Given the prevalence of bacterial biofilms in both native and engineered environments, our understanding of their interactions with both other bacteria and abiotic surfaces is quite limited. In this research we use an AFM to analyze the interactions of bacteria such as *E. coli* and a saprophytic, biofilm forming variant of *B. bacteriovorus* with other bacteria and chemically characterized surfaces. Tipless AFM cantilevers were left unmodified (Si3N4), or coated with a monolayer of *E. coli*. These cantilevers were then used to collect force curves on biofilms of *B. bacteriovorus* and *E.coli* as well as chemically characterized surfaces such as mica, silicon, and poly-L-lysine-coated glass. The greater the cantilever's contact time with the surface, the more force and energy was required to retract from the surface. *E. coli*-coated cantilevers had more adhesion to *B. bacteriovorus* biofilms than to *E. coli* biofilms, but even *E. coli - B. bacteriovorus* interaction paled in comparison to adhesion between *E. coli* biofilms and abiotic surfaces. Further results probing biofilms with cantilevers that have been chemically modified with acid or amine groups will be presented.

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A Self-Consistent Multiscale Methodology for Predicting Adhesion of Mammalian Cells onto Functionalized Surfaces

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Predicting cell adhesion onto surfaces functionalized with peptides is inherently a multiscale problem since the adhesion interface is mediated largely by interactions of specific peptides with surface receptors. This interaction occurs over length scales on the order of nanometers, while typical mammalian cells are on the order of microns. In this work, we showcase a self-consistent approach for obtaining specifics of interactions between peptide sequences and receptors, and then applying this chemical information to describe these interactions for cells that are decorated with these receptors. Using this approach we present adhesion equilibrium behavior for 3 different receptor-peptide sequences across a range of length scales, from 50 nm, to 500 nm. We believe this approach offers a clear path to scaling up to mammalian cells (5-20 microns).

3193-Pos Board B623

Mapping Interactions between Silver Nanoparticles and Biomolecules at the Atomic Level

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The association of biomolecules with silver nanoparticles (AgNPs) has been shown to modify the nanoparticles' stability as well as their behavior in the physiological environment. However, the details of how silver nanoparticle surfaces – replete with heterogeneities – interact with the equally heterogeneous surfaces of biomolecules remain elusive, yet essential to understanding the origin of the biological activity of AgNPs. Leveraging molecular dynamics simulation and free-energy/kinetics calculations, we have constructed maps detailing interactions of bare and functionalized AgNPs with peptides, proteins, and lipid bilayer membranes.

3194-Pos Board B624

Protein Corona and Secondary Structure in Response to Nanoparticle Pegylation

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Nanoparticles are versatile tools for biophysical applications. Using these particles requires a close examination of the protein corona: the layer of proteins that adsorbs onto the particle surface. Modifying nanoparticle surfaces with polyethylene glycol (PEG) has been shown to reduce corona formation. Because tightly bound 'hard' corona proteins can block surface ligands that could be used in targeting applications, a reduction in corona is desirable and can enhance our ability to effectively utilize nanoparticle surface modifications. First, gold nanoparticles were PEGylated and characterized with dynamic light scattering. Using gel electrophoresis, a three-fold decrease in corona formation was found for PEGylated nanoparticles compared to bare nanoparticles. With a reduction of corona confirmed, we next investigated the secondary structure of the corona proteins. PEGylated and bare nanoparticles were incubated with bovine serum albumin, the most prevalent serum protein. Using CD spectroscopy, we probed the secondary structure of the adsorbed albumin. Significant structural changes were not detected. In addition, bovine serum albumin, α2-macroglobulin, and transferrin were each incubated with free PEG. Once again, no alteration of protein secondary structures were found, even in the presence of a one hundred molar excess of free PEG. These results conclude that PEG can quantitatively reduce corona formation without altering structural aspects of corona proteins.

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A Theoretical Study of Polymer-Based Drug Delivery Systems

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A variety of interactions between drug delivery devices and local cells and tissues impact clinical outcomes in terms of both therapeutic action and biological response. Understanding the competition of interactions in highly inhomogeneous environments such as those relevant in tissue engineering, nanotechnology, and those responsible for biological cell function is critical to the further development of design platforms for delivery systems. We use a three dimensional mean-field theory to study the competition between electrostatic, van der Waals and steric interactions in determining the molecular organization of micelles made of ampliphilic diblock polybases designed to carry doxorubicin to cancer cells. The micelles are assumed to target cancer cells primarily through electrostatic binding as several cancers are known to flip negatively charged lipids to the outer-leaflet. The polyelectrolyte micelles spontaneously form self-assembled aggregates whose physical properties are manipulated by the composition of the solution in contact with the polymer system. These theoretical calculations show that chemical equilibrium and the relevant physical interactions present in responsive polymer micelless couple in such