Abstracts of Invited Talks

Prof. Michael Bartlett (Virginia Tech)
Title: *Soft Materials for Multifunctional Electronics, Robots, and Adhesives*
Abstract: Multifunctional soft materials and interfaces create intriguing new opportunities to enhance performance through programmable and adaptable properties. This talk will explore: 1) Solid-liquid soft composites for electronics, 2) Programmable adhesives for spatially selective adhesion, and 3) Morphing materials for soft robotics. I will highlight how liquid metal droplets embedded in elastomers create soft electronics with exceptional combinations of elasticity, electrical conductivity, and thermal properties. I will also discuss metamaterial adhesives that achieve strong, reversible, and spatially tunable adhesion by using programmed cut architectures to control crack propagation. Finally, I will introduce morphing materials that combine active materials with programmed geometry. This enables morphing materials to achieve reversible and lockable polymorphic reconfigurations, demonstrated in a soft robotic drone that autonomously transforms for multimodal locomotion. These approaches provide model systems to study fundamental material properties while enabling electronic skins, soft robots, and advanced adhesives for a variety of soft matter systems.
Speaker Bio: Michael Bartlett is an Associate Professor and John R. Jones III Faculty Fellow of Mechanical Engineering at Virginia Tech. His research focuses on soft multifunctional materials for deformable electronics and soft robotics, adaptive materials, and switchable and intelligent adhesives. He received his BSE in Materials Science and Engineering from Michigan in 2008 and Ph.D. in Polymer Science and Engineering from UMass Amherst in 2013. After obtaining his Ph.D. he worked as a Senior Research Engineer in the Corporate Research Laboratory at 3M, as a Postdoctoral Fellow at Carnegie Mellon University, and was an Assistant Professor at Iowa State University before joining Virginia Tech in 2020. His research has resulted in publications, patents, media coverage, and awards including an NSF CAREER award, a DARPA Young Faculty Award (YFA) and Director's Fellowship, a ONR Young Investigator (YIP) Award, a Senior Member of the National Academy of Inventors (NAI), the Early Career Scientist Award from the Adhesion Society, a 3M Non-Tenured Faculty Award, ASME Rising Star Award, and the Excellence in Research Award and Commercialization Champions Award from Virginia Tech among others.

Prof. Camille Bilodeau (Univ. Virginia)
Title: *Protein Adsorption to Peptide-Functionalized Surfaces: The Interplay Between Peptide Structure, Surface Morphology, and Protein Adsorption Strength*
Abstract: Charged and hydrophobic peptide-functionalized surfaces are widely used to regulate protein adsorption in applications such as tissue scaffolds, anti-biofouling coatings, protein separations, and drug delivery systems. While previous studies have shown that small changes in peptide sequence can significantly alter protein adsorption, these effects remain difficult to predict. Recent simulations suggest that peptide-peptide interactions can influence which residues are exposed to solvent and therefore available for protein binding. However, a clear understanding of how peptide structure determines presentation and ultimately protein adsorption is still lacking.

In this study, we combine molecular dynamics (MD) simulations and protein adsorption experiments to investigate how three key peptide design parameters, (1) the sequence order of hydrophobic and charged residues, (2) the spacing between these groups, and (3) the length of the linker attaching peptides to the surface, affect protein adsorption. Classical MD simulations reveal how these structural parameters alter peptide conformation and interactions between neighboring peptides, which in turn dictate which amino acid residues are solvent-exposed versus buried. Umbrella sampling calculations further quantify how these differences in surface presentation impact the free energy of protein adsorption. To validate these computational findings, we synthesized peptide libraries representing systematic variations in the three design

parameters and measured the adsorption of five model proteins under varying salt conditions. The experimental data closely match simulation predictions, confirming that peptide structure and presentation govern protein–surface interactions. This work demonstrates that subtle modifications in peptide design can induce measurable changes in surface morphology and protein binding behavior. Our results provide a mechanistic framework for predicting and tuning protein adsorption through rational design of peptide-functionalized surfaces, with broad implications for biomaterials engineering and surface science.

Speaker Bio: Dr. Camille Bilodeau is an Assistant Professor of Chemical Engineering at the University of Virginia. Her research integrates statistical thermodynamics, molecular simulations, and artificial intelligence to design new molecules and materials. She completed her Ph.D. at Rensselaer Polytechnic Institute with Shekhar Garde and Steve Cramer, followed by a postdoc at MIT with Klavs Jensen and Regina Barzilay. Dr. Bilodeau is a recipient of the NSF CAREER award and is involved in the scientific community through leadership roles in AIChE's Computational Molecular Science and Engineering, the Biotechnology Division of ACS, and the Gordon Research Conference on Water and Aqueous Solutions.

Prof. Daniel Beller (Johns Hopkins Univ.)

Title: *Braids, vortices, and twist lines in the topological defects of active nematics*

Abstract: From microtubule-kinesin suspensions to cellular tissues and bacterial colonies, a wide variety of biological and biomaterial systems share the behaviors of active nematics, which couple orientational order to internal force generation. Topological defects in the orientational order play essential roles in driving motion of the surrounding material. I will share recent progress from my research group in understanding the structure and dynamics of these defects. In strongly confined two-dimensional systems, we explore repeating cycles of defect motions that arise spontaneously (in a typically chaotic system) and trace out well-defined braids. We show how those braids are connected with the topology of vortex boundaries in the flow velocity field. Turning to three-dimensional systems, we find so-called twist disclinations—known from the study of liquid crystals—in the cell orientations of tumor tissue from gliomas, a form of brain cancer.

Speaker Bio: Daniel Beller is an assistant professor in the Department of Physics and Astronomy at Johns Hopkins University. He and his research group use theoretical and computational approaches to study a range of soft matter and biological systems with emergent, complex spatial structure. Previously, he was an assistant professor in the Department of Physics at the University of California, Merced. He obtained his Ph.D. in Physics at the University of Pennsylvania, and he worked as a postdoctoral researcher at Harvard and Brown Universities. He fell in love with soft matter physics as an undergraduate at Brandeis University.

Prof. Leah Spangler (Virginia Commonwealth University)

Title: *Engineering Proteins for the Biomanufacturing of Optoelectronic Nanomaterials*

Abstract: Biomineralization is a scalable, green, and sustainable method for producing a wide range of functional nanomaterials such as semiconductor quantum dots and metal nanoparticles. In contrast to traditional chemical approaches, biomineralization occurs under ambient temperatures and pressures using proteins or other biomolecules to drive synthesis. In the first part of my talk, I will demonstrate the synthesis of semiconductor quantum dots using a natural biomineralization pathway identified in the bacteria *Stenotrophomonas maltophila.* This biomineralization process was found to rely on a single enzyme, cystathionine g-lyase, which catalyzes nanocrystal growth by producing H_2S from the amino acid L-cysteine. Biomineralization was used to generate many types of semiconductor quantum dots including CdS, PbS, $CuInS_2$, $(CuInZn)S_2$ and the first reported fully biomineralized core/shell quantum dots, PbS/CdS and $CuInS_2$/ZnS. We demonstrate the application of these biomineralized nanoparticles in solar cells, fluorescent cell tagging, and photocatalysis.

In the second half of the presentation, I will demonstrate an alternative biomineralization approach which uses artificially designed *de novo* proteins. Natural biomineralization proteins are limited to certain types of materials (i.e. metal sulfides and metal oxides) because their synthesis relies on biochemical pathways that were initially evolved for biologically relevant materials. To expand the use of biomineralization to a wider range of relevant critical minerals, we have developed two *de novo* protein systems that can be tuned to produce a variety of inorganic materials for non-biological applications. *De novo* proteins are made by design using a binary polar-nonpolar amino acid motif resulting in high stability and facile tunability of protein function. Here, we demonstrate two *de novo* proteins developed for the controllable biomineralization of metal chalcogenide quantum dots. The first protein catalyzes the synthesis, while the second serves to template and stabilize nanocrystal growth. These systems are currently being engineered for the extraction and purification other materials, such as lithium hydroxides and rare earth elements.

<u>Speaker Bio</u>: Leah Spangler is an Assistant Professor of Chemical and Life Science Engineering at Virginia Commonwealth University. She obtained her Ph.D. in Chemical Engineering from Lehigh University where she studied the single enzyme biomineralization of semiconductor quantum dots for biomedical and energy applications. Leah then continued her research career as a Postdoctoral Research Associate in Prof. Gregory Scholes' lab in the Department of Chemistry at Princeton University where she studied the relationship between protein structure and optical properties of photosynthetic proteins. During that time, she also worked in Prof. Michael Hecht's lab studying de novo proteins for semiconductor nanoparticle synthesis. Leah's current research interests include engineering de novo proteins for applications in scalable material synthesis, rare-earth element separation, and optoelectronic systems.

Prof. Juan Cebral (George Mason University)

<u>Title</u>: *Blood Flow Dynamics and Cerebral Aneurysm Wall Structure*

<u>Abstract</u>: Brain aneurysms are pathological focal dilatations of the cerebral arteries which affect a significant portion of the general population (2-5%). Rupture of a cerebral aneurysm has devastating consequences with high mortality and morbidity. However, rupture of incidentally found asymptomatic aneurysms is quite rare. Nevertheless, preventive treatment is often recommended even though the risk of treatment complications may exceed the natural rupture risk. As such, precise assessment of aneurysm risk is very important to guide patient management. Current aneurysm evaluation relies mostly on patient characteristics (demographics, age, smoking, hypertension, family history, etc.) and very few aneurysm-specific characteristics (only size, location and presence of blebs). Thus, one of the goals of our research is to improve aneurysm evaluation and management through detailed understanding of the underlying mechanisms that drive the degradation of the aneurysm wall and its subsequent weakening and ultimately failure. In particular, blood flow is thought to play a central role inducing local structural changes to the wall which drive aneurysm evolution. Therefore, we develop and use patient-specific computational fluid dynamics models constructed from 3D medical images to investigate the effects of abnormal flow patterns on aneurysm walls by comparing hemodynamic features with data from multiple sources including clinical records, in-vivo imaging, and ex-vivo analysis of tissue samples resected during surgery. In this talk I will summarize some of our recent studies in this field.