MRL, PPG announce 2022 PPG MRL Assistantship Awardees

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Fufei An, Souvik Bhattacharya, Tarek Gebrael, Hyewon Jeong, and Luis Rodríguez Koett have been awarded PPG Materials Research Laboratory (MRL) Graduate Research Assistantships to pursue cutting-edge research broadly related to the areas of interest to PPG.

MRL director Paul Braun notes that PPG's generosity translates into a valuable opportunity for outstanding graduate students. "The PPG-MRL graduate research fellowship program gives top MRL graduate students the opportunity to propose and develop new areas of research and receive feedback from PPG scientists and engineers on their research, as well as opportunities to interact more deeply with PPG," he says.

Fufei An, Materials Science & Engineering (Qing Cao, Advisor)

An says, "My research is developing a new and unique strategy to synthesize amorphous materials at the 2D limit from solution-processable precursors. The process is scalable and can be repeated in a layer-by-layer fashion, allowing the production of multilayered films with atomically precise thickness over large areas for their application as transformative and novel insulators in various functional nanoelectronic devices, enabling unprecedented device performance and uniformity. The 2D amorphous carbon films are also attractive for applications such as catalyst supports and water purification membranes, with their unique heterogeneous and tunable atomic structures."

Qing Cao, An's advisor, states: "What really sets Fufei apart from her peers is her capability to complete the full innovation cycle, starting from the preparation of a new material, to understanding its unique properties and structure-property relationship based on a combination of experiment and simulation, and finally to finding its suitable engineering applications."

Souvik Bhattacharya, Nuclear, Plasma, & Radiological Engineering (R. Mohan Sankaran, Advisor)

Bhattacharya says, "The goal of my thesis research is to develop synthesis techniques for the production of large-area, thickness-controlled ultrathin films of materials that can serve as protective and functional coatings. The significance is that ultrathin materials have properties distinct from their bulk counterparts. There are currently two relatively well-established methods to obtain these materials: exfoliation from a bulk form, or deposition from vapors. Neither of these methods has yet been able to produce films over large areas and controlled thicknesses. To address this challenge, I am studying a new approach, which was established by me and another group member, termed 'plasma-enhanced chemical film conversion' or 'PECFC.' Briefly, this approach involves the conversion of a solution-cast film by a low-temperature plasma. The solution contains several components that can be mixed and matched, including a chemical precursor that is the source of the desired material, a polymer to bind the film when it is deposited, and a solvent to disperse the precursor and polymer. The solution can be deposited onto a substrate by a variety of methods, including printing to obtain patterns. Conversion of the precursor is achieved by the interaction of energetic and reactive species produced in a plasma, such as gaseous ions and radicals. Our approach has several potential advantages over exfoliation and vapor deposition. The material is deposited only where it is desired, thereby minimizing wastage and environmental impact. Furthermore, by utilizing plasmas to enhance our chemistry, we are able to move away from conventional furnace- or temperature-based synthesis methods which are far less energy-efficient and have a much larger carbon footprint. The solution-deposited films are continuous and scalable, and can lead to a conformal coating on a variety of substrates."

R. Mohan Sankaran, Bhattacharya's advisor, states: "Between knowing him as an undergraduate student researcher, and now as a graduate student, Souvik has deeply impressed me as one of the most independent, motivated, and skilled researchers I have ever had in my research group."

Tarek Gebrael, Mechanical Engineering (Nenad Miljkovic, Advisor)

Gebrael says, "Power densification of modern electronics is greatly shaped by emerging thermal management technologies. Dissipating the heat generated during operation is needed to keep the devices at temperatures below material limits. Powerful cooling methods, such as aggressive forced air convection relying on air handling units and chillers, can be costly. Therefore, engineers are constantly looking to implement more thermally efficient and cost-effective cooling techniques. Within this context, heat spreaders have proven to be an excellent choice. They spread heat generated inside hotspots and conduct it to a heat sink through an increased area, hence reducing thermal resistance. The two main limitations of the state-of-the-art approaches are as follows. (1) Heat spreaders are manufactured in a way that maximizes the contact area with hotspots, but in many devices, the location of the junction (the region where heat is generated) is unreachable by the heat spreader. (2) Heat spreader integration requires the application of a low-thermal-conductivity thermal interface material (TIM) between the mating surfaces to eliminate air gaps and provide mechanical compliance. To address the increase in thermal resistance due to those limitations, I developed a new method to grow a TIM-less copper spreader on electronics monolithically. The coating is conformal and covers all exposed surfaces, getting as close as possible to the junction of the device. In addition, since the coating eliminates air gaps at the interface with the mating surface, TIMs are eliminated."

Nenad Miljkovic, Gebrael's advisor, states: "While Tarek's scientific curiosity, eagerness to learn, and critical thinking have always led him to exciting findings, his scientific knowledge and rigor were always in place to explain these findings. His tenacity and patience were always helpful in tough moments during his research in my lab."

Hyewon Jeong, Materials Science & Engineering (Paul Braun, Advisor)

Jeong says, "Lithium-ion batteries (LIBs) have been extensively studied because of their ability to power portable electronics and electric vehicles. Efforts to maximize the capacity of LIBs are focused on the improvement of individual components, such as the cathode, electrolyte, and anode. Most LIBs contain graphite-based anodes, but graphite's theoretical specific capacity is only 372 mAh/g. Silicon, on the other hand, is a promising high-capacity anode material for LIBs. Its specific capacity is ten times higher than that of carbon-based anodes: 4200 mAh/g. It is also abundant in the Earth's crust, cost-effective, and environmentally benign. Despite its significant advantages, it has some drawbacks, such as volume expansion of up to 300% during charging, which leads to particle pulverization upon cycling. This further results in electrical contact loss and continuous solid electrolyte interphase (SEI) formation from the decomposition of electrolytes on fresh crack surfaces. To address these challenges, it is paramount to make a uniform and mechanically durable silicon coating on a current collector. Researchers in the field have devoted themselves to engineering silicon at different scales and dimensions. For example, silicon deposited on a 3D-architected nickel scaffold was designed to accommodate higher silicon loading and compensate for the volume expansion of silicon during lithiation. Nonetheless, the tortuosity in porous 3D structures adds complexity in understanding how silicon expands and the SEI forms on a highly curved surface. Some delamination of silicon also occurs in this tortuous structure, preventing silicon from being durable to extended cycling. My hypothesis is that study of the fundamental elements of the curvature of the 3D-structured geometry will give us an understanding of how each curvature element contributes to the chemo-mechanical properties of silicon. Then the SEI formation on curved silicon after cycling will be fundamentally understood. This study will also reveal the correlation between curvature chemistry and cycling stability."

Paul Braun, Jeong's advisor, states: "Hyewon is an outstanding graduate student and has proved herself worthy of the honor of a PPG-MRL fellowship by taking on several challenging projects on the study of interfaces and curvature on advanced materials for energy storage. Her project requires understanding of new materials deposition procedures, electrochemistry, and high-resolution electron microscopy. She is integrating her findings from across these methods to understand for the first time how curvature in thin films of energy storage materials and the atomic composition of interfaces in energy storage materials evolve with cycling."

Luis Rodríguez Koett, Materials Science & Engineering (Nancy Sottos, Advisor)

Rodríguez Koett says, "I propose to expand the frontal polymerization (FP) printing process by incorporating on-the-fly mixing techniques to manufacture materials with tailorable property gradients and functionality. This technique can then be used to manufacture a wide variety of materials, including coatings and composites. The proposed research plan is as follows. (1) *Development of a compatible on-the-fly mixing strategy:* Different strategies will be tested for mixing. These strategies must be compatible with the available printing systems at our disposal while ensuring proper mixing. A proof-of-concept will be shown by adding dyes into different monomers to test for homogeneous mixing. This setup will be tested

with inks of different compositions to ensure the robustness of the mixing technique. (2) *Controlled extrusion of material gradients:* A control system will be developed to allow manufacture of any arbitrary material gradient. Various gradients will be made by using a two-monomer system with soft and hard domains. The gradients will be probed with hardness and fracture tests to demonstrate advantages over monolithic materials. (3) *Manufacturing of multifunctional tailored materials:* Functional materials like self-reporting microcapsules will be incorporated into the material as it is extruded. This will further test the robustness of the mixing strategy and control system. Manufactured materials will be damaged at predetermined regions to probe the survival of the capsules during the mixing and extrusion. Microscopy techniques will be used to examine sample cross-sections and estimate the volume fraction of microcapsules successfully introduced. The proposed work will lay the foundation for development of a robust on-demand functional material manufacturing technique that draws inspiration from PPG's MoonWalk system. Such a technique would allow users to design a material with an arbitrary property gradient and functionality and have a direct way of manufacturing such a material."

Nancy Sottos, Rodríguez Koett's advisor, states: "Luis has extraordinary potential for conducting impactful research, combined with a passion for science and education. I believe his proposed research has potential to be transformative and provide a new approach to processing materials with complex morphology and function with energy-efficiency and scalability far beyond current manufacturing methods."

About the PPG Assistantships

To help build the next generation of diverse STEM leaders, PPG and the PPG Foundation support talented students pursuing their post-secondary studies, ensuring they have the tools and resources they need to be successful. The PPG Foundation also partners with leading universities to establish launching points for a diverse STEM talent pipeline and the world-class expertise and discovery that make tomorrow's possibilities a reality. The PPG Foundation is entering its sixth year of partnership with the University of Illinois, including funding of the MRL Graduate Research Assistantships, which support students and the University community with new thought leaders at the MRL. The company invested $13.3 million in community engagement programs in 2021, including more than $6.6 million invested globally in education.

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