LEADERSHIP & IMPACT

MULTIFUNCTIONAL MATERIALS INTEGRATION
HIGH-ENTROPY ALLOYS
2-D MATERIALS
ADDITIVE MANUFACTURING
MESSAGE FROM THE CHAIR

This year, our department’s accomplishments position us to continue to grow and lead in focused areas of materials science beyond the next decade. Our recent, prestigious, peer-reviewed publications illustrate the quality of our faculty and the high impact of their research. Jimmy Burns, Kyusang Lee (joint ECE/MSE), and Haydn Wadley, as well as incoming faculty member Prasanna Balachandran (joint MSE/MAE), had noteworthy scientific manuscripts appear in Nature publications, including one featured on the cover.

We have added three new faculty hires, which reinforce our expertise in computational materials science and data informatics, as well as in fabricating and characterizing high-performance multifunctional materials based on complex oxides and other compounds. Their presence will enrich the department across the board and reinforce our strong role in UVA Engineering’s Multifunctional Materials Integration initiative.

This year was also significant in that we attracted several million dollars in external research awards for instrumentation. This enabled us to grow our programs in the materials science of surfaces and interfaces and especially to acquire surface characterization equipment. We also updated and expanded our suite of nanoscale characterization equipment, thanks to a multimillion dollar grant and faculty start-up funds from the University.

Taken together, these initiatives enable the department to launch exciting collaborative projects— in multi-functional integration, high-entropy alloys, 2-D materials, and additive manufacturing—that will advance the engineered materials world and serve society.

JOHN R. SCULLY
THE CHARLES HENDERSON CHAIRED PROFESSOR AND INTERIM CHAIR
Assistant Professor Stephen McDonnell's research focuses on understanding how 2-D materials, such as the transition metal dichalcogenide family, interface with other materials in electronic devices. Understanding the bonding in interface heterostructures is crucial to enabling the engineering required to integrate materials into nanoelectronic device architectures.

In his lab, McDonnell has established a dedicated ultra-high vacuum growth and characterization system that allows him not only to synthesize high purity 2-D semiconductors, but also to investigate the structure, composition, and electronic properties of these materials without any atmospheric exposure. This capability has fostered a number of collaborations at UVA. McDonnell is working with Associate Professor Patrick Hopkins to understand the correlation between metal-semiconductor interface chemistry and both electron and phonon transport across these interfaces. They have found that interface chemistry can have a dramatic effect on thermal transport (see accompanying figure).

The ability to investigate interfaces and also to synthesize 2-D materials has led to a new collaboration with Assistant Professor Mona Zebarjadi. Theoretical models suggest that 2-D materials may enable a new generation of thermoelectric devices. McDonnell has also been collaborating with Professor Giovanni Zangari to investigate the surface chemistry evolution during photoelectrochemical water splitting. Their work has included the integration of graphene as a barrier layer to protect cost-effective silicon photoanodes during operation.

By controlling the oxygen composition in titanium contacts to graphene we can vary the thermal boundary conductance (TBC). The left panel shows the X-ray photoelectron spectroscopy (XPS) of four sample titanium contacts. XPS is used to quantify the chemical composition of the sample and shows the varying Ti and TiO$_2$ content. The right panel shows the resultant change in TBC as determined by time domain thermal reflectance.

By controlling the oxygen composition in titanium contacts to graphene we can vary the thermal boundary conductance (TBC). The left panel shows the X-ray photoelectron spectroscopy (XPS) of four sample titanium contacts. XPS is used to quantify the chemical composition of the sample and shows the varying Ti and TiO$_2$ content. The right panel shows the resultant change in TBC as determined by time domain thermal reflectance.

By controlling the oxygen composition in titanium contacts to graphene we can vary the thermal boundary conductance (TBC). The left panel shows the X-ray photoelectron spectroscopy (XPS) of four sample titanium contacts. XPS is used to quantify the chemical composition of the sample and shows the varying Ti and TiO$_2$ content. The right panel shows the resultant change in TBC as determined by time domain thermal reflectance.

By controlling the oxygen composition in titanium contacts to graphene we can vary the thermal boundary conductance (TBC). The left panel shows the X-ray photoelectron spectroscopy (XPS) of four sample titanium contacts. XPS is used to quantify the chemical composition of the sample and shows the varying Ti and TiO$_2$ content. The right panel shows the resultant change in TBC as determined by time domain thermal reflectance.
Two of the most exciting fields to emerge in materials science and engineering in recent years are additive manufacturing and high-entropy alloys. By building on its existing strengths, UVA is developing distinctive approaches in both areas to help realize their potential.

One obstacle to widespread use of 3-D printed metals is the effect on materials' microstructure given the continuous welding inherent in the process. This is particularly an issue with aluminum alloys, but it is also a factor in austenitic stainless steels, which are subject to grain boundary sensitization and subsequent intergranular corrosion. Not all of the consequences of these welds can be determined through mechanical process testing that has been the focus of most work elsewhere, but are only revealed over time.

Because of the department’s world-class research programs in time-dependent processes—corrosion, fatigue and oxidation—that the Office of Naval Research called on Professor Rob Kelly to evaluate the corrosion susceptibility of 3-D printed 316L and 625 corrosion resistant alloys, both mainstays of marine construction. Members of Kelly’s lab have already found evidence that parts printed with 316L exhibit sensitization in the as-printed condition, something that does not occur with material made using standard processes.

UVA faculty are also developing strategies to address these issues. Under the auspices of the Naval Surface Warfare Center, Dahlgren, Professor Sean Agnew and Associate Professor Jim Fitz-Gerald are determining whether laser surface treatment of 3-D printed metals can mitigate such time-dependent processes. In addition, Professor Haydn Wadley, in a collaboration with GE Additive Solutions, is exploring ways in which additive manufacturing can be used to significantly enhance the performance of cellular materials made from titanium alloys.

Another way in which the department is extending its expertise into new areas is high-entropy alloys. In the 13 years since these multiple principal element systems were first reported, researchers have developed a number of equiatomic alloys with heretofore irreconcilable properties, including alloys that are both strong and ductile. The major impediment to their systematic development is the absence of phase diagrams for such multicomponent systems, combined with the lack of fundamental modeling/simulation tools to predict microstructure evolution and the relationship of microstructure to specific properties.

To help solve this problem, the department is bringing to bear expertise in thermodynamics, metallurgy and simulation. Faculty members such as Wadley are collaborating with colleagues at other universities to secure funding to develop better simulation tools, and the department is actively reinforcing this expertise by recruiting faculty members specializing in relevant modeling methods. Professor John Scully, interim department chair, is designing improved corrosion-resistant alloys by using the tailored compositions and structures promised with high-entropy alloys as part of a prestigious DOE Energy Frontier Research Center where Scully leads the metals team.

Ultimately, growing programs in additive manufacturing and high-entropy alloys will position the UVA Department of Materials Science & Engineering to help lead in the development of 21st century structural materials.
Since the invention of the transistor 50 years ago, advances in computing have been swept along on a river of silicon. As the most common material for semiconductors, silicon has many advantages, not the least of which is its abundance. But at last that stream is beginning to slow as manufacturers and researchers reach the limits of silicon’s physical and chemical properties.

Finding successors for semiconductor materials like silicon and the interfaces between these materials is the goal of UVA Engineering’s Multifunctional Materials Integration initiative, with the Materials Science & Engineering Department playing a leading role. The initiative includes more than 40 faculty members from across various disciplines.

“At UVA, we have expertise, spanning individual departments and schools, to begin reinventing the information age and to take this research from atoms to applications,” said Patrick Hopkins, one of the leaders of the initiative, associate professor of mechanical and aerospace engineering with a courtesy appointment in the Materials Science & Engineering Department. Hopkins last year won the U.S. government’s highest honor for early career scientists and engineers for his work on nanoscale energy transport.

The purpose of the initiative is not simply to replace standard semiconductor materials and interfaces but to find even better ones that offer higher energy efficiency and as yet unachievable performance and functionality. Such designer materials could set the stage for advances in such varied areas as 5G wireless networks, hardware for the Internet of Things, high-density data storage and artificial vision.

“Advances in new and energy efficient technology cannot be achieved anymore by insular thinking but require cross-disciplinary collaboration,” said Petra Reinke, associate professor of materials science and engineering. Professor Leonid Zhigilei, also a founding member of the initiative, agrees. “A unique characteristic of the multi-functional materials integration initiative is its highly interdisciplinary nature, which pushes us out of the comfort zone of our disciplinary areas of expertise and, at the same time, enables a broad range of very promising collaborative activities.”

The School of Engineering is hiring cross-cutting research faculty for the initiative, including:

Jon Ihlefeld, jointly appointed to the Materials Science & Engineering and Electrical & Computer Engineering departments. Ihlefeld joins UVA from Sandia National Laboratories, where he was a distinguished member of the technical staff of the Electronic, Optical and Nano Materials Department. Ihlefeld recently earned the 2017 Richard M. Fulrath Award from The American Ceramics Society for his contributions to electronic ceramics research and development.

Nikhil Shukla, jointly appointed to the Electrical & Computer Engineering and Materials Science & Engineering departments. Shukla joins UVA following Ph.D. studies in electrical engineering at the University of Notre Dame.
The International Journal of Materials Research presented its 2017 Werner Koestler Award for the best paper published in the journal during the preceding year to Research Scientist Liang Don and University Professor Haydn Wadley.

The National Science Foundation selected Assistant Professor Mona Zebarjadi for a prestigious CAREER Award. Zebarjadi will design solid-state power generators suitable to work under large temperature differences, setting the stage for widespread commercialization of solid-state power generators.

Assistant Professor Kyusang Lee was part of a team that has devised a way to use remote epitaxy to produce flexible films, preparing the way for heterointegration in photonics and flexible electronics. Their article was featured on the cover of Nature.

The MSE department expects to grow its T3 ranks from 19 in 2016 to 25 by the end of 2017.

Thanks to funding from the University of Virginia, the department will see the installation of $2.5 million in research equipment in 2017, including a Helios GU4 focused ion-beam SEM, a FEI/TFS Themis Z Scanning TEM, Versaprobe III XPS, a PANalytical Empyrean theta-theta X-ray diffractometer (XRD), and a PANalytical Epsilon 3X X-ray fluorescence (XRF) system.