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Quentarius Moore almost left chemistry after he finished his undergraduate degree at Mississippi’s Jackson State University. He initially hoped to attend graduate school in chemical engineering, but those plans fell apart. His grandmother had died earlier that spring, and Moore spent the following summer working in his grandfather’s concrete-finishing business.

Moore mulled his options with a friend, Christopher Copeland, who was a chemistry graduate student at the time. Copeland encouraged him to come back to Jackson State and pursue a master’s degree. “Just see what happens,” Copeland said.

Moore returned to computational chemistry research and hasn’t looked back. The Department of Energy Computational Science Graduate Fellowship (DOE CSGF) recipient, now at Texas A&M University, uses simulation tools to probe mechanochemistry — how physical force influences molecular reactions.

Curiosity, fearlessness and supportive mentors have guided Quentarius Moore’s scientific journey. Today he simulates how mechanical force can alter chemical reactions in materials.
His science interests date back to watching *Mythbusters* on the Discovery Channel as a teenager. Moore liked the puzzle of mathematics and chemistry and seeing how everyday processes work. “I wanted something that was quintessentially hard,” he says. “I liked the challenge of it.”

As a freshman, Moore joined a peer-mentoring program that matched him with a junior and a graduate student who worked in computational chemistry and gave Moore his first taste of the subject. Moore also tried experimental research on nanoparticles. In 2014, he grew two-dimensional chemical films while in a National Science Foundation summer research program at the University of Alabama. His advisor, Hung-Ta Wang, also urged him to go to graduate school.

Two years later, that summer research project helped Moore connect with his future Ph.D. advisor, James Batteas. They met at a conference where Moore described listening to Bruno Mars while coaxing molybdenum disulfide (MoS$_2$) films to grow in Wang’s lab. After the talk, Batteas and Moore discussed music, mutual science interests and Moore’s future. Batteas and his colleagues were launching a project on MoS$_2$, and he thought Moore’s computational expertise would be a key asset. “We have all these big ideas,” Batteas told Moore, “and I think you could be the right person for this.” Moore visited Texas A&M for several weeks that summer and explored research in Batteas’ group before applying to the Ph.D. program in 2017.

Chemists have carefully studied how light, heat and electricity affect chemical reactions, Moore says. But “we don’t understand how force alters reaction energy and pathways,” factors that are important as researchers consider solid lubricants. The atomic and nanoscale jagged edges on these surfaces can cause wear and tear or make them vulnerable to chemical reactions such as oxidation. The research also has implications for devices that must function in extreme environments. “If you shoot a satellite into space and you want something to actuate and it doesn’t actuate, that’s a big problem.”

Moore studies two-dimensional systems such as graphene – carbon in sheet form. Its surface is known for being relatively inert, but graphene lubricants demonstrate reactivity under wear and tear. Defects and pokes that bend the surface out of plane can cause the carbon atoms to react with free-radical molecules. The MoS$_2$ work includes computational materials scientists at Sandia National Laboratories in New Mexico, where Moore has completed two practicums with Michael Chandross. MoS$_2$ can work well as a solid lubricant, Chandross says, but exposing it to water and air can drastically increase friction. Composite coatings can help overcome this problem, but so far it’s unclear how and why they work, which limits their use. So the team’s focus is helping researchers understand these chemical details to help build better lubricants.

When Moore arrived at Texas A&M, he had used only density functional theory (DFT), a computationally intensive tool that can become too demanding when simulating a large number of atoms. Through his Sandia research, he learned a molecular dynamics method, LAMMPS, that lets researchers probe larger periodic systems such as graphene and MoS$_2$ while including approximations. More recently he’s incorporated plane-wave DFT, a technique that offers advantages of both approaches, into his research.

Moore is the lone computational chemist in Batteas’ group, where other researchers use atomic-scale microscopes to probe chemical surfaces. Moore plans to do experiments, too, which would provide new insights for his computational work. For example, he thinks that artificial intelligence methods offer an opportunity to glean new details from the Batteas group’s extensive experimental datasets that follow chemical reactions occurring on surfaces. The group recently received a
$1.8 million National Science Foundation grant to found a center, with the University of California, Merced, the University of Pennsylvania and others, for research, outreach and entrepreneurship focused on mechanochemistry. Moore is a key link within the center’s computational work, Batteas notes, collaborating with researchers at other institutions to set up simulations.

“Quentarius is one of the hardest-working Ph.D. students that I’ve ever had,” Batteas says, but he remains relaxed, even when working through stressful situations. “He’s a really calming force in the lab.” Moore also injects fun into what could be routine tasks, such as organizing the group’s regular research meetings. Recently he assigned lab members to two teams and modeled the meeting structure after the popular video game *Among Us*. “Nothing with him is boring,” Batteas says. Chandross appreciates Moore’s independence, attention to detail and grasp of the big picture. “He’s eager to learn and is also unafraid.”

Moore has helped with Texas A&M’s annual chemistry open house, and he plans to continue that outreach while building resources for chemistry instruction back in Mississippi. He had few childhood science role models, he says, and wants future generations to see the full range of such career opportunities.

Moore’s longtime interest in photography and videography could support those projects. While at Jackson State, he freelanced for ESPN, providing technical support for Division I college football games in Alabama, Mississippi and Louisiana and at Memphis bowl games. Much of the work involved running along the sidelines and supporting camera operators as they got action shots. He reprised that role for a 2019 Texas A&M game.

Chandross has arranged for Moore to become a Sandia intern, allowing him to split his time between New Mexico and Texas until he finishes his degree in 2022. Moore is exploring a range of research career options. The DOE CSGF program of study was difficult yet rewarding and increased his interest in computer graphics, visualization and statistical techniques, he says. “The CSGF hasn’t narrowed my career choices but instead blossomed my interests to be more than I ever expected.”

# CLEVER CLIMATE

**Benjamin Toms’** Lawrence Berkeley National Laboratory practicum with Karthik Kashinath and Prabhat inspired him to refocus his Ph.D. research, with Colorado State University’s Elizabeth Barnes, to machine learning for climate predictions. They combined physical theories about how ocean patterns affect precipitation and temperature and incorporated them into neural networks. “Then we try to understand what the neural network has learned so we can learn something new about the system itself,” Toms says. He and his colleagues believe they can predict near-term climate, up to several years ahead. He’s launched a company to build models for that purpose.

# (QU)BIT PLAYER

**Annie Wei’s** Massachusetts Institute of Technology (MIT) quantum algorithm research unites her interests in computer science and physics. Her methods are designed to run on quantum computers that use qubits, computer bit equivalents that also can represent both one and zero simultaneously, boosting computational power and efficiency. But today’s quantum computers are small and error-prone, so Wei often uses HPC systems to simulate quantum algorithms. She’s built techniques to solve several problems, including analyzing mountains of data from giant particle accelerators. Wei also creates methods with both classical and quantum-mechanical parts to employ the best features of each kind of computer.

Molybdenum disulfide can form sheets with two distinct crystal patterns: 1H, which acts like a metal; and 1T, which acts like a semiconductor. Combining these two in a single device could help with the design of new electronic devices. This image overlays Quentarius Moore’s calculations of these structures on microscope images from the Batteas group.

Credit: Quentarius Moore and Michael Chandross.