Scientific Modeling:

Our Scientists in Portrait

2015

Mark Gordon is a distinguished professor of chemistry whose research uses computing to understand the behavior of atoms and molecules. He and many collaborators developed the General Atomic and Molecular Electronic Structure System, or GAMESS, a software program designed to run on supercomputing systems to model complex physical, chemical, and biological systems.

“I was a graduate student with the Nobel Prize-winning theoretical chemist John Pople’s research group in 1964. He told us that we should learn computer programming, and then promptly left for summer vacation. By the time he came back in the fall, we were pretty good at it.”

Matt Kramer is a materials scientist who studies the structures and properties of glass-forming, intermetallic, and high-temperature alloys and permanent magnets through electron microscopy and high-energy X-ray diffraction.

“I’m perpetually intrigued by the beauty in the complexity and symmetry of materials when looking through the electron microscope. I am like the eye in the sky. I can tell experimentalists ‘yes, you did,’ or ‘no, you didn’t’ reach the goal in producing a certain material with the desired structure. Better yet is being able to say ‘you made something new and unexpected.’”

Anja Mudring, a scientist in solid state chemistry, researches the properties and applications of ionic liquids, which are room-temperature molten salts. Ionic liquids have many potential uses as environmentally friendly solvents, in materials synthesis for phosphors and nanoparticles for catalysis, and in the recovery of rare-earth metals.

“Most salts don’t burn, so neither does ionic liquids. That makes them ideal as substitutes in traditionally toxic processes. And their unique properties mean that we can fine-tune them to meet a lot of different purposes.”

Ikenna Nlebedim's research is on magnetism and magnetic materials. Since joining Ames Laboratory in 2010, he has studied oxide-based magnetic, magnetostrictive and magnetoelectric materials, magnetic nondestructive evaluation, and magnetic topological insulators. His current research in the Critical Materials Institute includes development of substitute materials for strong permanent magnets and improving the reuse and recycling of rare-earth permanent magnets.

"We can help to ensure the energy security of the United States by integrating the ability to discover and make powerful permanent magnets with the smartness to make them more efficiently and the wisdom to recycle them where we can."

Durga Paudyal works in theoretical condensed matter physics, researching the electronic structure and magnetic properties of rare-earth and transition-metal based materials. His interest in developing computational models of new materials exhibiting new and unusual physical properties could lead to innovations in areas such as computing and renewable energy.

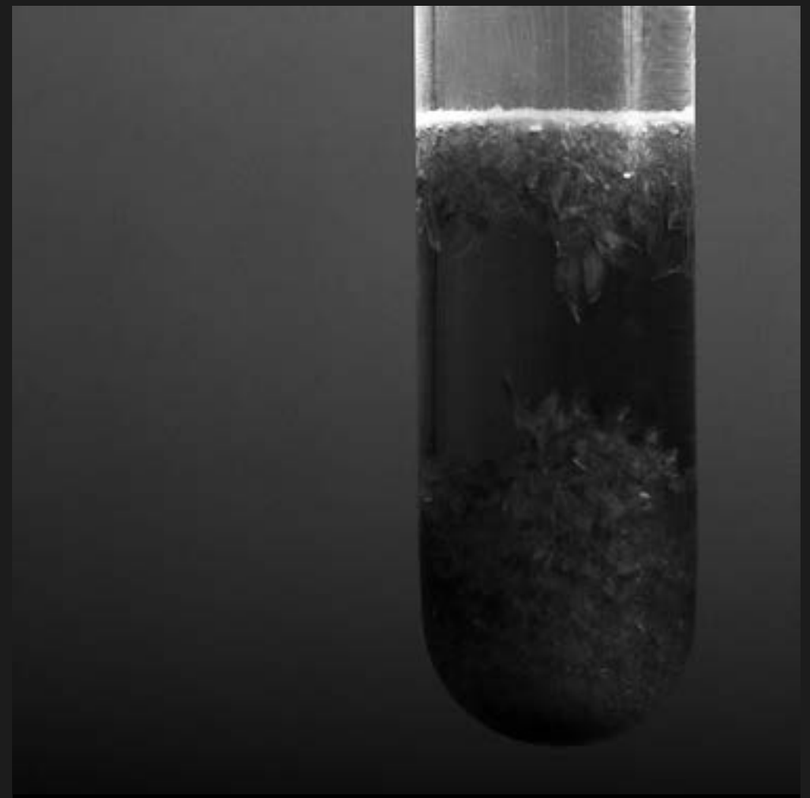
“Theorists and experimentalists are no use to each other working separately. But working together, we can design superior and highly useful materials more quickly.”

Ruslan Prozorov is a low-temperature condensed matter physicist with research interests in experimental superconductivity, magnetism, nano- and meso-scale science, and pattern formation in complex electronic systems. He develops advanced instrumentation and measurement techniques necessary to probe quantum mechanical properties of complex materials.

“Magnetism is fascinating because this invisible force has pure quantum mechanical origin, yet can be experienced in everyday life. Even understanding the science behind it, it seems like magic to me still.”

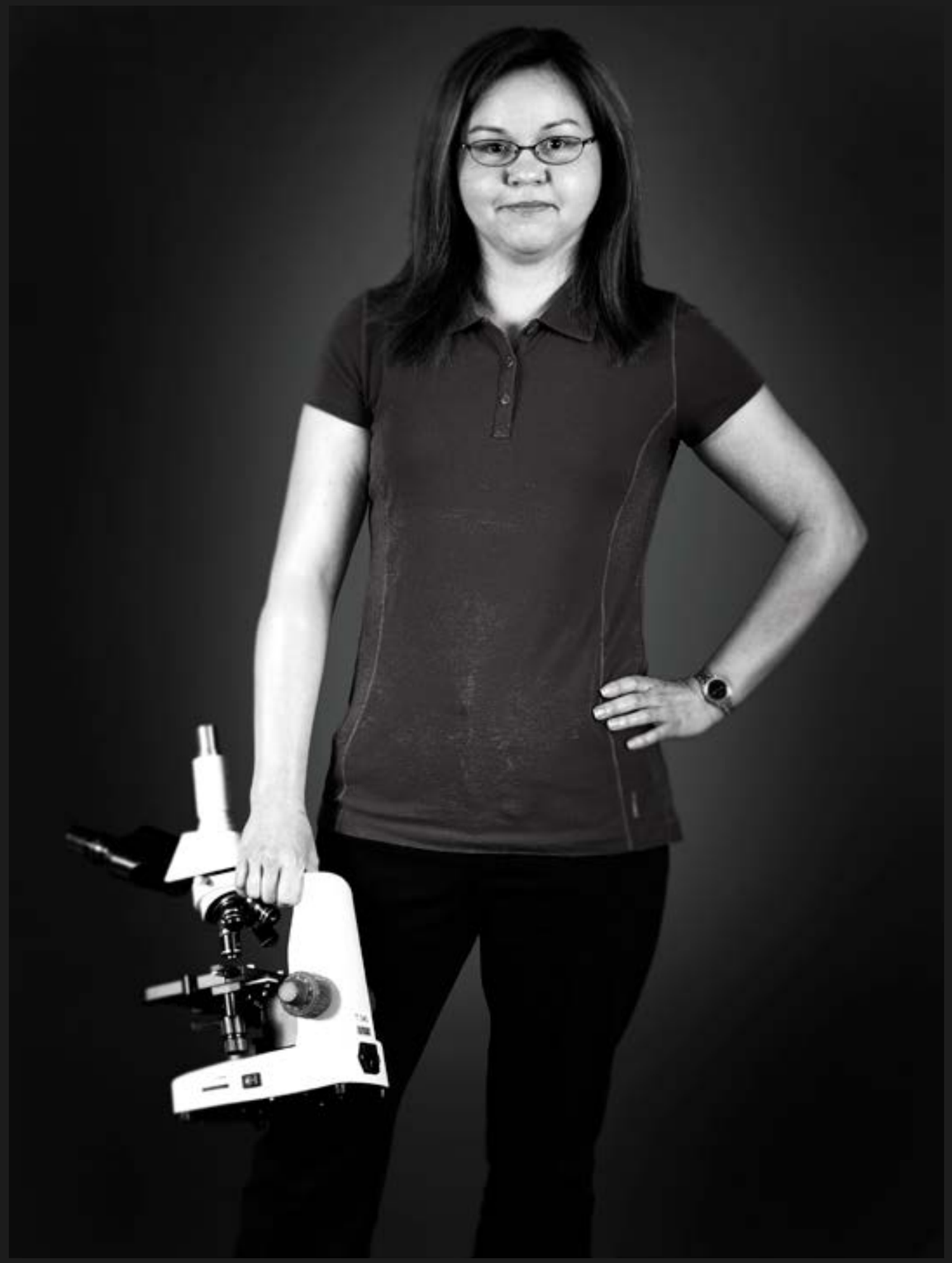
Tanya Prozorov investigates how magnetotactic bacteria produce chains of magnetite crystals within their cells, using liquid cell scanning transmission electron microscopy. Her research goal is to understand the mechanism of formation and growth of magnetic nanocrystals by these microorganisms, so new materials mimicking these tiny biological magnets can be created in the lab.

“I like solving puzzles, and I want to know how a single cell organism does a superior job creating nanometer-sized magnets. I am a materials chemist who uses advanced microscopy to understand and learn how things work.”



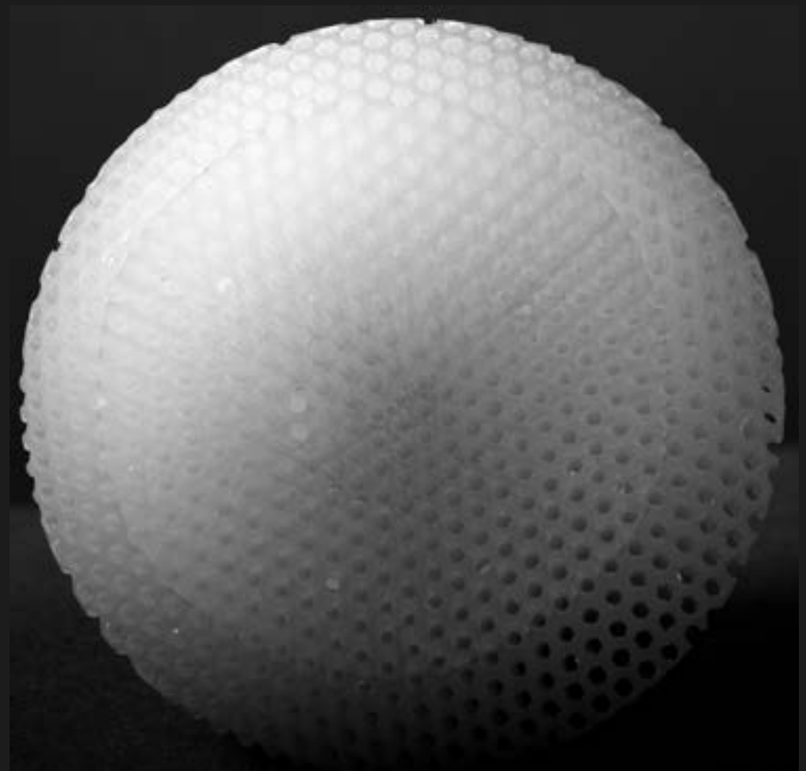
Aaron Sadow is a scientist in the Chemical and Biological Sciences Division. He investigates the use of organometallic compounds as catalysts for chemical, material, and energy-related synthesis.

“Chemistry is about making molecules. I like being able to hold up a vial and know that no one has ever connected atoms in that way before; there’s an inherent fascination in creating something new and understanding how it works.”



Emily Smith came to Ames Laboratory in 2006 via Northwestern University, Penn State, University of Wisconsin-Madison, University of Delaware and University of Arizona. She's involved in the development of instruments such as fluorescence and Raman scattering imaging to analyze everything from biomass to new materials for solar cells.

"I'm an instrument builder. My team is currently building equipment to study thin films that have uses in solar energy. I would measure my success by having solar panels outside my home one day that used technology my team helped develop."



Igor Slowing joined Ames Laboratory in 2009 and develops multi-functional nano- and meso-scale particles for catalysis. His research in the synthesis of these structures and in understanding and controlling their chemical properties has applications in fields as diverse as manufacturing, biofuels production, environmental remediation and sensing.

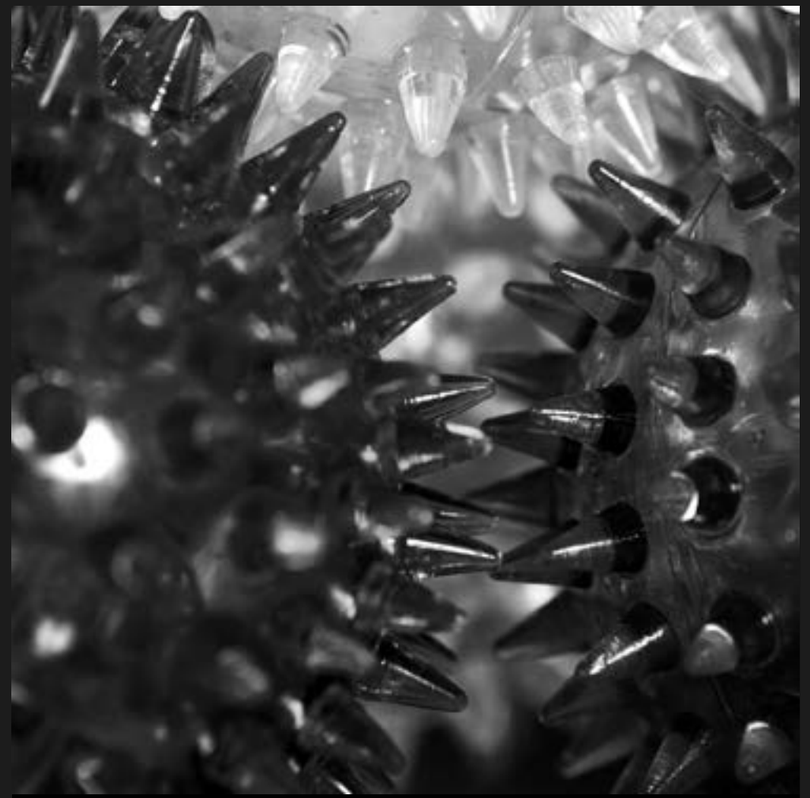
“Nanostructures are like a playground for a scientist. There are so many ways you can arrange and modify them and so many tasks they can accomplish, the limit is only your imagination.”

Chris Strasburg is a computer systems analyst. He develops sophisticated algorithms to manage information, to monitor for and defend against cyber-attacks, and to protect the nation's energy infrastructure.

"The idea that you can teach computer systems to learn from data is endlessly intriguing; it gives us the power to automate complex activities that humans don't like or find difficult to do."

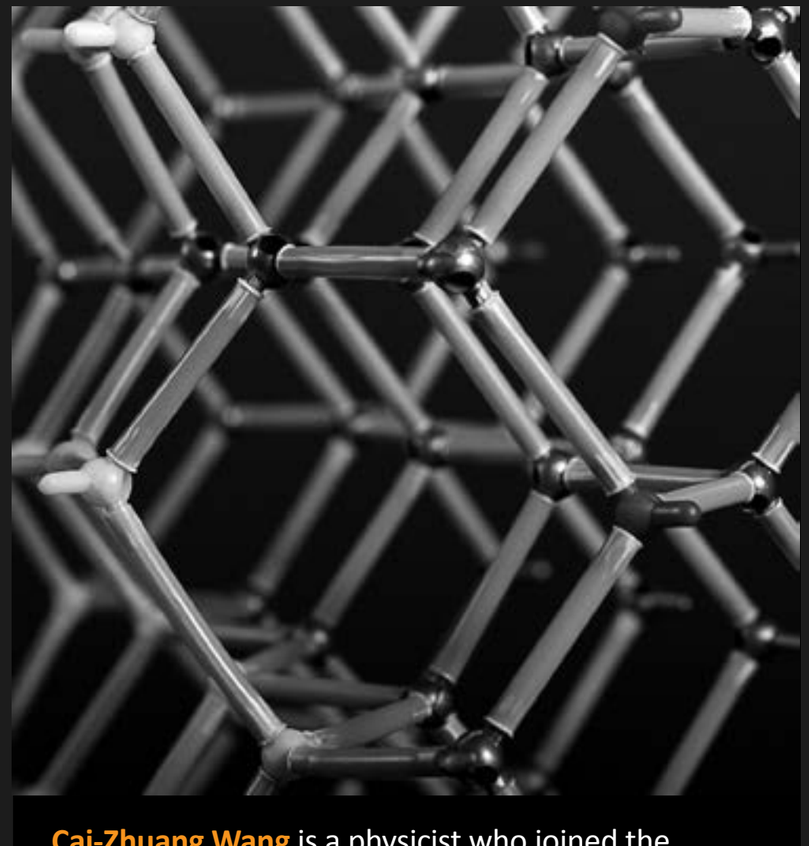
Pat Thiel is an award-winning physical chemist who investigates the surface structures and properties of complex systems such as quasicrystals or nanoparticles on metal and semiconductor surfaces.

"Nature is so much smarter than we can ever be, even on a good day. Over and over again we'll uncover something that is initially astonishing, but then after intense investigation and modeling, we realize, 'Oh, of course, it must be that way.'"



Javier Vela is a scientist with the Laboratory's Division of Chemical and Biological Sciences. His work focuses on photoactive nanomaterials for applications in catalysis, renewable energy, and biological imaging. He also researches the synthesis, functionalization, and bottom-up directed assembly of semiconductor and metal nanocrystals.

"Physicist Richard Feynman once said 'there's plenty of room at the bottom,' meaning that there was lots of unexplored capability to manipulate materials at the atomic level. It turns out he was right. Nano-science is a whole new frontier."



Cai-Zhuang Wang is a physicist who joined the Ames Laboratory in 1987. He creates computational models and simulations of the structural, electronic, and phase transformation properties of condensed matter systems and molecules.

“Computational models speed up the process of materials discovery. Through modeling, we can sort through a great amount of complex data and narrow down the possibilities to material compositions that are most likely to have the properties we are seeking.”

Linlin Wang is a physicist who specializes in the computational design of nanoscale alloys and magnetic materials. Through modeling and simulation, he investigates the electronic structure, thermodynamics, kinetics, and catalytic properties of new materials.

“Physics is the ultimate understanding of how things work; and in computational physics there is so much freedom to explore systems and change parameters that understanding and materials design can happen more quickly.”

Photographer Shauna Stephenson is a 2005 graduate of Iowa State University's Greenlee School of Journalism. She lives and works in Montana, and is the northwest regional communications director for Trout Unlimited, a non-profit conservation organization. As a Public Affairs student intern, she shot the first series of hallway portraits that have been on display on the first floor of TASF since 2005.