the chemists club

spring 2013

THE UNIVERSITY OF CHICAGO

Team work

Alumna Nancy Forde brings UChicago's interdisciplinary spirit to her molecular research.

By Claire Zulkey

If there's one thing Nancy Forde, SM'95, PhD'99, came away with from her time at the University of Chicago, it's that science can be a team sport—literally. "We had a very good women's intramural basketball team from chemistry and physics," says Forde, associate professor of physics at Simon Fraser University. "There were some very competitive women in the chemistry department, and they recruited heavily. I had only played basketball in gym class before that, but we won the University championship twice, beating the undergrads. It was really fun."

Continued from cover:

Team work

Such camaraderie didn't take place only on the basketball court. "The interdisciplinary interactions at Chicago were really good, both scientifically and socially," says Forde, whose lab was in the James Franck Institute. "I interacted with a lot of people in physics and chemistry. When you get to know people personally, it makes it a lot easier to talk to them scientifically."

These crosscurrents have remained present in Forde's work. After researching biological molecular motors for her postdoctorate at the University of California, Berkeley, she joined British Columbia's Simon Fraser University in 2004. She's now part of an international collaboration striving to predict the motor properties revealed when the team assembles proteins or nucleic acids in different ways. "We're working toward this common goal that no one's ever done before, which is to make a molecular motor out of proteins."

After they learn about molecular construction and how new properties emerge, they hope to create nanoscale devices utilizing motor transport—for example, chips for diagnostic assays. Lead project investigator Heiner Linke, now at Lund University in Sweden, asked Forde to join the collaboration because of her background with DNA and optical tweezers. "Then my role evolved," she says. "My chemistry training from Chicago helped with appreciating the importance of understanding the chemical kinetics of interactions."

Although the team is far flung, including principal investigators from four different disciplines located in Europe, Canada, and Australia, "this particular collaboration has been absolutely fantastic," says Forde. "We see things from different perspectives, but we've had annual meetings to come together for a few days and just brainstorm."

Forde believes in sharing knowledge on her home turf as well. In fall 2012 she helped organize the inaugural President's Dream Colloquium series at Simon Fraser University, presenting a seminar course on the emergence and complexity of life. Topics included: How might life have emerged on earth? What is the earliest evidence we have for life on earth? How can complexity emerge from simpler levels of organization? "We had students from eight different departments interspersed with invited speakers," she says. "A large portion of the course was getting people to communicate with each other, to be able to appreciate the literature appropriately and convey deep ideas and the overall relevance to the broader group."

This winter Forde's molecular-motors team wrapped up some proof-of-principle experiments to send to their Swedish collaborators for measurements as they looked into getting another grant. Meanwhile she is studying how collagen and elastin self-assemble from individual proteins into high-order structures. "What is it about the chemical changes that give rise to the mechanical changes?" she explains. "We're trying to understand this correlation by starting at the molecular level."

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This work is facilitated by the same collegial atmosphere that Forde found in her UChicago days. "I screen people before they're admitted to my group," she says. "I ask them about how they think about science and get a feel for their personality. It's a small group, so while they don't have to be best friends, they do have to respect each other and work well together."

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CHEMISTRY EVENTS The calendar of named lectures for the 2012–13 academic year, as well as the most up-to-date information about Department of Chemistry lectures and events, can be found online at event.uchicago.edu/chem/index.php.

LET'S KEEP IN TOUCH The Department of Chemistry is updating its records. Send your current e-mail address and other contact information to Tanya Shpigel at chemistsclub@uchicago.edu.

Forest for the trees

Graduate student James Dama develops simple models to study complex molecular systems.

By Jeanie Chung

When he was in high school, James Dama couldn't decide whether he ultimately wanted to study philosophy or bioengineering. "In the end, I decided that if I were doing bioengineering, a lot of philosophy would be in there too," he says. "A lot of theory of abstraction."

He attended Caltech but maintained a philosophical outlook there and in his graduate studies at UChicago. As a third-year PhD candidate and one of five graduate students with Professor Greg Voth's Center for Multiscale Theory and Simulation, Dama focuses on coarse-graining methodologies, a topic he explains this way: "If you understand something at a fine-grained level—if you can see all the trees—how do you figure out the forest?"

Working at the center, Dama developed a new theory called ultra-coarse-graining that, according to Voth, "promises to revolutionize our ability to computationally explore and understand the behavior of biomolecular and other complex condensed-phase molecular systems."

As an example of ultra-coarse-graining, Dama cites the work Voth's group is doing with HIV. "We have an understanding of the quantum mechanics that make all the individual atoms move," he says. "And we have an understanding of the structure of the HIV virus. So if we can put all the atoms in place—in theory—and then figure out the quantum mechanics, we can just start making the atoms move [to learn to defeat the virus]. It would all be correct in theory, but the problem is that, to do that, the quantum mechanics is so complicated that it takes much longer than we have to live. You would never save anyone."

Instead, Dama uses computational simulation to help researchers develop simpler, abstracted models of the virus, then use those abstracted models to discover how the virus works. Dama refers to it as "redefining the stuff you study in chemistry."

"Really, this is no different from what we do in our daily lives," he says. "Just take it down to the essentials. The problem is, in this case, we don't usually know what the essentials are, so it's our job to come up with general principles for distilling models down to their essentials."

Voth notes that Dama has a few more years of work to do on his PhD, "and I expect many more discoveries will come from his brain before leaving us." At that point, Dama is unsure of his next step, noting that coarse-graining simulation has applications far beyond computational chemistry, and that, while he enjoys working in Voth's group, he is not necessarily set on a career in academia.

"I have a brother in high-speed finance, and we can talk about each other's work very well," he says. "I might like to go into something more industrial."

Dama keeps up with philosophy and has attended campus lectures on Wittgenstein and Heidegger, among others. He embraces the opportunity to live the life of the mind—and "to be around a lot of people who feel the same way."

It's a world far from what he envisioned growing up in northern Florida, where he figured he would go to a state school and then perhaps a career in the military. "When you're outside of [academic] circles, things look very, very different than when you're inside them," he says. "It's easy to get into negatives and think that you don't belong."

Now that he's proven he does belong, Dama hopes to be an example. The center has done outreach to high school students, and he describes a visit to Lane Tech High School in Chicago as "one of the coolest things we did."

The main message he hopes to convey to these students? "People outside of these circles shouldn't sell themselves short."

Synthesized success

A passion sparked in the College burns bright in the middle of a stellar career.

By Sean Carr, AB'90

Jonas Peters, SB'93, has green hands.

"It means you can make new things," explains Peters, the Bren professor of chemistry at Caltech. "Inorganic and organometallic synthesis requires a degree of dexterity, an ability to manipulate complex glassware, that I really enjoy."

That's pretty much the only thing you'll hear Peters brag about. He's quick to thank his parents and several mentors for supporting and guiding him down the path that has led to a quick rise in his field and a long, continuing string of honors.

Others are less reticent to praise Peters. "His research has been pretty spectacular," says Greg Hillhouse, in whose lab Peters worked as an undergraduate, including a year on a prestigious Goldwater Fellowship. "He's made some fundamental discoveries concerning iron," including its possible role as a pathway to biological nitrogen fixation—"one of the holy grails of synthetic chemistry."

Peters, in turn, says Hillhouse remains an incredible mentor and that his UChicago lab experiences helped him discover the work that became a passion and has unfolded into his life's pursuit.

"The first time I made a new molecule in Hillhouse's lab was a pretty exciting event," Peters says. "Creating a new type of matter—it didn't matter what—was a thrill. There's a lot of craft to it." He also explored chemistry's theoretical side, modeling coordination complexes with the department's then chair, the late Jeremy Burdett. After graduating, Peters spent a year in the United Kingdom on a Marshall Scholarship, working with Burdett's doctoral adviser, James J. Turner, at the University of Nottingham.

"He was an amazing adviser," Peters says, "and that was an intellectually satisfying, broadening experience—in ways well beyond chemistry." At the same time, a year doing laser spectroscopy reminded him how much he had missed chemical synthesis. Says Peters, "That's when I made the very conscious decision that I like the craft of synthetic lab work better."

He returned to the States in fall 1994 to begin doctoral studies in inorganic chemistry at MIT under Professor Christopher C. Cummins, focusing on the use of low-coordinate tris-amido molybdenum and

“He’s made some fundamental discoveries concerning iron,” including its possible role as a pathway to biological nitrogen fixation—“one of the holy grails of synthetic chemistry.”

titanium complexes to activate and functionalize small molecules. He graduated in 1998 with a job waiting for him in Caltech’s division of chemistry and chemical engineering, but first he spent a postdoctoral year as a Miller Fellow at the University of California, Berkeley, with T. Don Tilley.

In Pasadena Peters met his match: Dianne Newman, who was carving out several niches at Caltech as a geomicrobiologist. They married in 2003, and four years later both accepted offers at MIT. But Caltech wasn’t giving up and in 2010 welcomed Peters and Newman—and by that point, their young son—back to the West Coast.

Today Peters and his group are attacking several problems, including the use of widely available metals, like nickel and cobalt, as hydrogen-evolution catalysts in solar-fuels systems. “We’ve also gotten some really cool results on Fe-mediated nitrogen fixation recently,” he says. For the latter work, his lab has even attracted funding from the National Institutes of Health.

Several research contributors in his lab include College alumni who, after working with Hillhouse and others, have joined Peters’s group as grad students. “I am clearly biased,” Peters says, “but the U of C turns out some great undergrads in chemistry.”

Chemistry’s future, it seems, is in good—green—hands.

FROM THE LABS

The Department of Chemistry has received a prestigious GAANN grant from the US Department of Education, supporting six graduate fellowships per year, from 2012 through 2015, for students who demonstrate financial need and plan to pursue the highest degree available in fields designated as areas of national need.

Gregory Voth, the Haig P. Papazian distinguished service professor, has won the 2013 American Chemical Society Physical Chemistry Division Award in theoretical chemistry, recognizing his contributions in developing and applying new theoretical and computational methods in the study of biomolecules, liquids, materials, and quantum mechanical systems.

Professor Gregory Hillhouse also has won the American Chemical Society Award, in Organometallic Chemistry, for his contributions to synthetic and mechanistic organometallic chemistry. Please read more about Greg’s work in this issue’s faculty interview.

Assistant professor **Bozhi Tian**, in addition to receiving a 2013 National Science Foundation CAREER Award (see the chair’s letter), also was selected as a 2013 Searle Scholar. Earlier he was named a TR35 honoree from MIT’s *Technology Review*, identifying the world’s top innovators under age 35 in emerging fields of science and technology.

Marking the 80th birthdays of three UChicago chemists, a meeting this past September, dubbed the “240 Conference,” drew more than 120 colleagues to Kent Lab. The conference, devoted to chemical physics, honored **R. Stephen Berry**, the James Franck distinguished service professor emeritus in chemistry; **Joshua Jortner**, professor emeritus of chemistry at Tel Aviv University; and **Stuart Rice**, the Frank P. Hixon distinguished service professor emeritus in chemistry.

The Department of Chemistry will hold its second annual Industrial Associates Meeting May 1. The professional-development and networking event brings together 10–12 researchers in industry with graduate students and postdocs for a condensed recruiting experience. In addition to matching students and potential employers, the meeting exposes students to industrial career paths.

Link with us

The Department of Chemistry encourages all alumni to connect with current chemistry students and each other on LinkedIn. The department’s group, called the University of Chicago Department of Chemistry Network, can be found at tinyurl.com/7efp2t2. Feel free to post questions for discussion and add your own two cents in comments. The more students and alums who interact, the more useful the group will be.

Faculty interview:

Gregory Hillhouse

(From the Fall 2012 *Inquiry*)

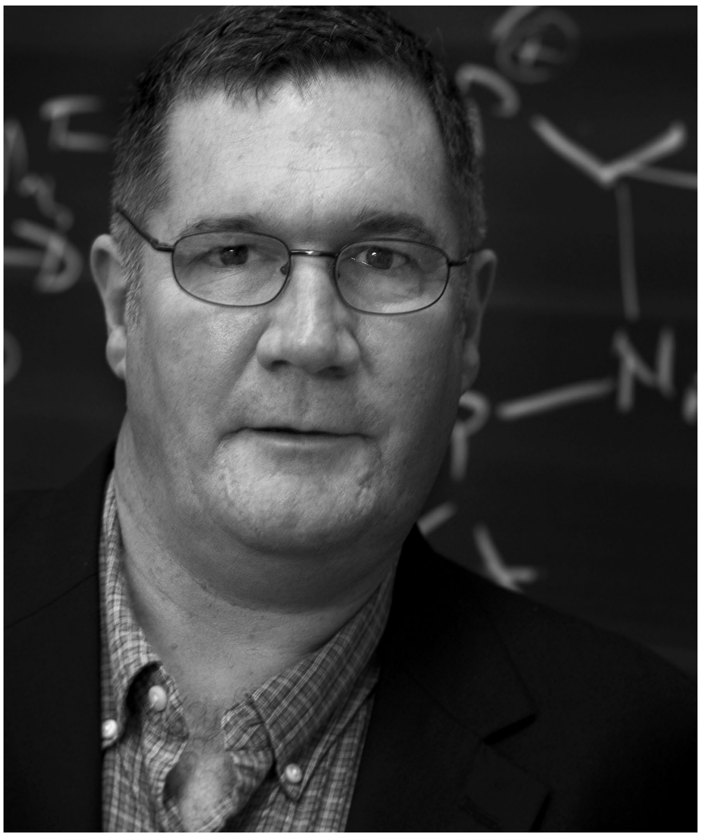
Gregory Hillhouse, professor of chemistry, is a synthetic organometallic chemist. Hillhouse, who joined the Chicago faculty in 1983, won a Quantrell Award for his undergraduate teaching in 1997 and a Norman Maclean Faculty Award in 2011 for his mentorship of undergraduates. More recently he won the 2013 American Chemical Society Award in Organometallic Chemistry.

What he does

Hillhouse's primary research interest lies in finding new ways to create multiple bondings with late transition metals—groups 9 and 10 on the periodic table, such as nickel, cobalt, palladium, and platinum—and studying their reaction chemistry. "The ultimate goal is to take one fragment from a molecule and then add it to another small molecule," he explains. "Maybe you take a nitrogen fragment, maybe a nitrene fragment, from an organic azide and add it to an olefin to make an aziridine. Or take nitrous oxide, which is very available and a good source of an oxygen atom, and add that to another organic molecule to undergo a very specific oxidation."

Why precious metals are doubly precious for him

The late metals aren't just for decoration. "They carry out many catalytic processes, like forming carbon-carbon bonds and hydrogenation," he explains. They have a range of uses outside the lab too, which is why cars' catalytic converters contain platinum (and why thieves try to steal them).



The geometry of chemistry

In transition-metal chemistry, the coordination number reflects how many neighbors the molecule's central atom has. A lower coordination number makes it easier for that molecule to create a bond. Typically a group 10 metal has a coordination number 4. As Hillhouse explains, "If you have four ligands, there are two common ways of arranging them around the metal: a tetrahedron and a square plane. Because of the orbitals that are required, those define the electronic structure of the metal." A tetrahedron structure has two unpaired electrons, and a square planar arrangement has none, meaning there are no orbitals available to form a multiple bond. However, "If you move the ligands, you can reduce the coordination geometry from four-coordinate to three-coordinate. Now there are orbitals available for forming the double bond." Hillhouse's group recently pushed forward into two-coordinate geometry, which opens up a new set of possibilities for reactions.

On being first

Hillhouse's group was the first to prepare multiple bonds with late transition metals a decade ago. "Many people thought they couldn't be prepared," he says, for "good reasons—mainly that for certain coordination geometries, they couldn't." Today there are many groups worldwide doing it. "It's quite popular."

His favorite molecule

"My current favorite one would have to be a two-coordinate nitrene complex that we recently reported," he says. "Since that one got us to coordination number 2, that's probably my favorite molecule."

If there was one thing he could do with his career

Hillhouse would like to make a late transition metal bind to an oxygen atom. "That would be a very attractive intermediate. It should have very useful reactivity in synthesis for these oxygen-transfer processes," he says. "Many have been reported, and they've all been wrong."

On working with young people

Hillhouse won the Maclean Faculty Award for mentoring undergraduate students. (His research group currently has as many undergraduates as grad students.) "It's nice to see the kindling of a spark of interest in the first- or second-year undergraduates and watch that mature into a successful scientific career."

He works with undergrads outside the lab too: he's a big supporter of the University's athletic department. "They need some mentorship from faculty, so I've served in that role for quite a few years. The sports teams are fighting an uphill battle, and the faculty don't cut them any slack."

Congratulations

AB and SB recipients

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Damon Wang

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Linzi Wu

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Mijo Simunovic
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the chemists club

Spring 2013

Dear friends,

In the sciences it's important to give students excellent course training and also to expose them to state-of-the-art research opportunities. We are making several new efforts to achieve these goals, starting with renovating the undergraduate labs for organic chemistry labs and later for general chemistry. We also have installed a new clean room in Searle for micro and nanofabrication to support research in materials, biophysics, and other areas.

We have hired two faculty members this year. Andrew Tokmakoff, the Henry G. Gale distinguished service professor in chemistry and the 2012 winner of the American Physical Society's Ernest Plyler Prize, comes from MIT to tackle new biological problems using ultrafast vibrational spectroscopy. Also from MIT is assistant professor Bozhi Tian. Tian won a 2013 National Science Foundation CAREER Award, which he will use to investigate "the fundamental limits of signal transduction at the interface between biological cells and inorganic materials." The Tokmakoff and Tian research groups will occupy newly outfitted lab space in GCIS.

We have long emphasized research as a key element in our undergraduates program, and we encourage students to attend chemistry conferences, meet people in the field, and present their work. We now have a way of funding such trips, thanks to a generous gift. The Gordon A. Nobel Travel Fund supports student travel to present research results.

During the past year two intellectual leaders have retired from the faculty. Hisashi Yamamoto, the Arthur Holly Compton distinguished service professor of chemistry and the College, came to UChicago in 2002. Specializing in the chemistry of catalysts that help to trigger or drive asymmetric molecular reactions, in 2009 he won Japan's Grand Prize of Synthetic Organic Chemistry, among other accolades. Also retiring is Karl Freed, the Henry J. Gale distinguished service professor in chemistry and the College. Joining the University in 1968, Freed is a fellow of the American Academy of Arts and Sciences and of the American Physical Society. His group has made advances in the statistical thermodynamics of polymers, protein dynamics, and molecular electronic structure. Both of these colleagues will be sorely missed.

We welcome new spaces and faces, congratulate and thank our longtime colleagues, and, with your help, continue to strive toward our goals.

Best Regards,

Richard F. Jordan
Professor and Chair