

## Fulbright Award will take Researcher to “Land Down Under”

*Mark Gordon to spend four months in Australia*

“I wouldn’t know what to do with myself if I wasn’t doing research,” says Mark Gordon. “I get up in the morning thinking about science, and I go to bed at night thinking about science.”

It’s good he feels that way because Gordon, director of the Applied Mathematics and Computational Sciences Program and an ISU Distinguished Professor in Liberal Arts and Sciences, will have plenty of science to think about in the upcoming months. A Fulbright Award will take him to the Australian National University in Canberra for a February-through-May, four-month sojourn. While there, he’ll be collaborating with three ANU colleagues on separate research projects.

Gordon’s passion and the focus of most of his waking moments is quantum chemistry — a branch of physical chemistry that deals with explaining chemical phenomena by using the laws of quantum mechanics. Consequently, two of his ANU collaborations will be with Leon Radom and Michael Collins, who both conduct research similar to Gordon’s.

In one effort, Gordon and Radom will be working on a new quantum chemistry method to predict the thermodynamic properties of complex systems, such as transition metal compounds, excited states and metastable species. Pioneering work in the prediction of thermodynamic properties for simpler organic molecules was done by Nobel Laureate John Pople, who was both Gordon’s thesis advisor and Radom’s postdoctoral advisor.

“It turns out that Pople’s methods are not appropriate for some complex systems,” says Gordon. “In chemical reactions, there are some species called reactive intermediates that are very important in chemistry, but

you can’t really ‘grab’ at them — it’s hard to measure them experimentally. They don’t hang around long enough to do measurements on things like heat of formation, ionization potential or spectroscopic properties. So theory is very important.”

In order to predict the thermodynamic properties of more complicated chemical species as well as the Pople methods do for simple organic ones, Gordon says you have to use more sophisticated methods, and therein lies the problem. Although he and Radom have recently developed the first method applicable to more complex systems, its high level of sophistication still limits the size of the system to which it can be applied.

“The method works really well — the error bars are as good as they are for the Pople method,” says Gordon. “But,” he muses, “can we come up with a clever way of extending this to much bigger chemical systems than it can be applied to right now?” That will be just one challenge in Gordon’s Australian adventure.

Another research endeavor will involve working to merge GROW, a quantum chemistry code developed by Collins, with the GAMESS program developed by Gordon and Ames Lab associate scientist Mike Schmidt. “GAMESS is a program that does quantum chemistry electronic structure calculations,” says Gordon. “Using GAMESS, we can predict properties of molecules and we can look at chemical reactions and predict barriers to reactions and the mechanisms by which reactions occur.”

Gordon notes that Collins’ work is in microscale dynamics and that the GROW program actually grows the potential energy surfaces for systems containing four to seven atoms. He explains, “If you knew the



*Mark Gordon*

energy as a function of all the possible ways that you could arrange all the atoms, then you could take that information and figure out how the available energy in a chemical reaction is distributed among the products and how the products are behaving as a function of time. Generating the potential energy surface is a tremendous problem,” continues Gordon, “but GROW is a very clever program that does this automatically by telling GAMESS the points at which it wants an energy calculated.”

The third research collaboration made possible by Gordon’s Fulbright Award will be with Alistair Rendell in ANU’s computer science department. “Alistair has a background in parallel quantum chemistry — very high-performance quantum chemistry,” says Gordon. “We’ll be working on developing more parallel code for GAMESS that will be some combination of graphics and parallel programming.”

In addition to the three research collaborations, Gordon will also be giving invited talks at

ANU, Sydney University, the University of Melbourne and Hobart University in Tasmania. But just in case this heavy-duty pace doesn’t provide enough science to satisfy his soul, he’ll get an extra dose on a side trip to South Korea. “The Fulbright is a great deal,” he states. “Since I’m going to what is called the Asia-Pacific area, I can apply for Fulbright funds to visit one other Asian country.” While in South Korea, Gordon will visit two of his former postdocs and give invited talks at the South Korean Chemical Association and two universities in Seoul.

Looking forward to his lengthy stay in Australia doing what he loves best, Gordon says, “It’s fun to go. For the most part, I can think just about science for four months. It’s like getting to go to the World Series all the time,” adds the avid baseball fan, who will actually save a week in his busy schedule to vacation in New Zealand. “I’ve never been there,” he says. “Of course, part of my motivation is that I have a colleague there.” Go figure! ■

*~ Saren Johnston*