Jeff Greeley

This year, Argonne materials scientist Jeff Greeley received an Early Career Research Award from the Department of Energy. Below, Jeff shares some thoughts about the trajectory of his research and his long-lasting relationship with scientific inquiry:

How did you get interested in science in the first place?

I credit my early interest in science to my mom and dad. They both have scientific backgrounds: my dad is a medical doctor and my mom is a research immunologist. They were always encouraging me as I was growing up to discuss scientific issues and chat about interesting science news that they had heard. My dad subscribes to Discover and Science, so those magazines were always lying around the house through the time I was in high school. So I think both of them encouraged a culture of scientific curiosity and creativity—they certainly didn’t force me into a scientific career but they didn’t discourage it by any means either.

When I was in high school I had a couple of very good teachers as well—both a great chemistry teacher and a great physics teacher. I think that kind of early education is very important in getting people to move into scientific careers.

How did you explore your early interest in chemical engineering?

When I started my undergraduate degree at UT-Austin, I was pretty sure I wanted to go into engineering, which is what I ultimately did. For a very brief time at the beginning of my freshman year, I was oscillating between aerospace engineering and chemical engineering. But I decided I wanted to pursue chemical engineering because it had more of the chemistry and physics flavor to it, which were fields I was interested in.

Engineering at the undergraduate level has an interesting mixture of a purely scientific component and an applied industrial component, and that’s what engineering as a profession is set up to be. I decided I was more interested in focusing on the scientific component as a career. My professors in Austin essentially told me that at the graduate level there was very little difference between chemical engineering and chemistry, and I think that’s true. They said I might as well just continue to get my Ph.D. in chemical engineering, and so that’s essentially what I did. I went on to UW-Madison for graduate school and got involved with a pioneer in the field of chemical reactions on metal surfaces, and the rest is history.

Why is doing computational chemistry and making electronic structure calculations valuable?

The great power of these simulation techniques is that you can take them and make predictions of the energies of specific configurations of atoms that have very few

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adjustable parameters. So, even when we know very little about a system to start with, we can actually make some predictions about how stable certain configurations are or how energetically favorable it is for a certain chemical reaction to occur. Alternatively, we can look at how changing the structure of a catalyst can change the properties of a catalyst or battery or fuel cell in which it’s used. The technique is very versatile—it’s like a molecular playground for scientists to enjoy.

How has the field changed since you started out as a graduate student?

In the past ten years or so, several changes have occurred. People are now able to look at much more complex reaction chemistries. Through one of the Energy Frontier Research Centers here at Argonne, we’re able to look at chemical reactivity of biomass on metal surfaces—those are pretty large molecules with lots of different reaction pathways and hundreds of different reaction intermediates. That’s really the state of the art for that kind of research these days—it’s gotten much richer in terms of the reaction networks than what was previously possible.

Also, when I started out, there were only relatively modest computer clusters available—roughly ten to twenty computers per cluster. That was typical for a normal academic group. You could still do interesting research and look at interesting problems, but you had to be much more selective in the kinds of systems you wanted to consider. We’d have to consider just one or two specific systems or look at simple molecules on surfaces, so there was less flexibility in a sense.

Another change is that people have begun to develop enormous databases of computational results. So the idea is that instead of just storing the hundreds or maybe a thousand calculations that you’ve done over a year or two, you have the results of hundreds of thousands of calculations in a database so you can actually do data mining to look for new patterns and trends that you weren’t able to do before.

Which challenges do you find the most interesting in your work?

On the general level, what I really like about this kind of work is the ability to get down into the details of what happens on the atomic level. In all of those application areas—the electrochemistry, catalysis, batteries and energy storage, being able to understand the details of the atomic processes—how particular chemical reactions take place on a surface or in a nanoparticle, or in the case of batteries how lithium ions make their way into and change the structure of anodes and change the capacity of a battery—I find all of these processes to be fascinating at the atomic level.

At the same time, even though I enjoy thinking about things at the very small scale, it’s really satisfying that all of these areas have very useful applications. The catalysis work is almost entirely based around processes that the chemical industry is currently using in one way or another. There’s a lot of industrial interest in the work that we’ve been doing.

What does the Early Career Award mean to you?

The Early Career Award is both humbling and exciting at the same time. It’s a tremendous opportunity to explore some new research avenues, over a period of several years, that I would not have been able to study otherwise. As part of that work, I intend to study some of the aspects of electrocatalysis and heterogeneous catalysis at solid/liquid interfaces.