Communicating Research to the General Public

At the March 5, 2010 UW-Madison Chemistry Department Colloquium, Prof. Bassam Z. Shakhashiri, the director of the Wisconsin Initiative for Science Literacy (WISL), encouraged all UW-Madison chemistry Ph.D. candidates to include a chapter in their Ph.D. thesis communicating their research to non-specialists. The goal is to explain the candidate's scholarly research and its significance to a wider audience that includes family members, friends, civic groups, newspaper reporters, program officers at appropriate funding agencies, state legislators, and members of the U.S. Congress.

Over 20 Ph.D. degree recipients have successfully completed their theses and included such a chapter.

WISL encourages the inclusion of such chapters in all Ph.D. theses everywhere through the cooperation of Ph.D. candidates and their mentors. WISL is now offering additional awards of $250 for UW-Madison chemistry Ph.D. candidates.

Wisconsin Initiative for Science Literacy

The dual mission of the Wisconsin Initiative for Science Literacy is to promote literacy in science, mathematics and technology among the general public and to attract future generations to careers in research, teaching and public service.

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May 2014

Timescales of Large Amplitude Motion - Classical and Quantum Considerations

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A dissertation submitted in partial fulfillment of
the requirements for the degree of

Doctor of Philosophy
(Chemistry)

at the
UNIVERSITY OF WISCONSIN-MADISON
2014

Date of final oral examination: 10/30/14

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Introduction for broader audience

I welcome the initiative by the Wisconsin Initiative of for Science Literacy to include a chapter in my thesis to convey the work I have done to non-specialists. I have adopted the style of a dialogue between the reader and myself for this chapter to overcome the monotony of long paragraphs. I, like most scientists, love talking about my research and this chapter is partly based on conversations I had over the years about my research with several friends.

Q. What branch of chemistry do you study?

I am a physical chemist. This branch uses our knowledge of physics to better understand chemical reactions. Specifically, I am a theoretician, who attempts to simulate chemical reactions on computers as well as develop theories that have experimentally verifiable predictions.

Q. Can you summarize your thesis as if you are describing it your grandmother?

Wow, that's exactly the question asked to me in my visa interview. My thesis comprises two projects. First, I study a phenomenon found in nature called tunneling. It is so bizarre that we do not have any direct physical experience of it. Imagine hitting a baseball with a bat, and imagine a full head-on collision. Well the ball will bounce back from the bat, right? Almost always! It turns out that if you follow the laws of quantum mechanics, a theory developed in the last century, there exists a very, very small probability that the ball will pass right through the bat. These probabilities are much larger at atomic scales.

Q. Why is tunneling relevant?

Implications of tunneling can be seen all around us. Consider the sun, where energy is created by fusing together hydrogen atoms. Even the sun does not have enough energy to surmount the huge repulsion that the two positively charged nuclei feel, and bring them close enough to fuse. The hydrogen atom tunnels through the repulsion barrier, leading to fusion. Radioactivity is also a consequence of tunneling. There are several examples in biological systems as well where tunneling is crucial. DNA, the basic ingredient of life, has two strands that are connected through 'hydrogen bonds'.

Sometimes hydrogen tunnels from one strand to another, which is believed to be the cause of certain diseases as well as aging.

Q. Can you be specific about what tunneling is?

Tunneling occurs when a particle passes through a 'barrier' without ever being at the barrier. This barrier is whatever makes two things interact or feel each other. In the case of baseball, it is the collision of the atoms of the baseball with the atoms of the bat. In the sun, it is the electrostatic interaction between the protons. For DNA, it is the forces responsible for the hydrogen bond.

Q. So a particle can go from one place to another, without ever passing through regions in between. Is that possible?

That is a very interesting question, and has puzzled many, including me. The short answer is that quantum mechanics predict it, and people have observed this phenomenon by constructing very careful experiments. Hence it must be. Sir Arthur Canon Doyle in one of his novels said 'When you have eliminated the impossible, whatever remains, however improbable, must be the truth'.

In quantum mechanics, matter can act as both particle and wave. That is strange, but a thoroughly verified fact. When you think of a wave, it is not really 'present' at any one point, but spread out. It is possible to imagine a situation where this wave can have a large amplitude on one side of the barrier initially, and a large amplitude on the other side at a later time.

Q. What exactly do you study about tunneling?

Tunneling, as I mentioned earlier, can be important in many biological systems. Yet we do not know how to include its effects in conventional large scale simulations, which have become an indispensable tool in chemistry. I have investigated a mathematical model, involving only a few variables, that describes proton tunneling. As the proton tunnels, the surrounding atoms and bonds reorganize which can have profound effects on tunneling. I employ the model with the aim to develop new methods, as well as improve existing ones, to include the reorganization effects on tunneling in the large scale simulations. The small number of variables simplify equations that describe tunneling, greatly helping in development of new methods, as well as providing a deeper understanding of tunneling.

Q. What are the key results of this project?

A very interesting feature I discovered is that under certain conditions, the reorganization of the surrounding atoms can increase the time it takes for the proton to tunnel. I tested two of the most promising methods available for large scale simulations, and observed that they miss this feature. I suggested improvements in one of them. It remains to be seen if this improvement will work for larger, and more complex, systems. I further tested another method, that is somewhat specifically designed for this particular mathematical model. This method works reasonably well, and includes all the features to some degree.

I also developed a method of my own. This new method works extremely well for the model I have studied. Although more work will be required to include this method in large scale simulations.

Q. Please briefly describe the other project you have worked on.

In my second project, I investigate the flow of energy in molecules. Imagine a cup of hot tea left out. After a while, it will cool down to the room temperature. Something similar happens in molecules. Any chemical reaction requires energy. When the products of the reaction form, this energy dissipates away by a process known as vibrational energy relaxation. I have studied in detail the time it takes for the molecule to cool down.

Q. Why do you care about how much time it takes for energy to dissipate?

When the product of the reaction forms, it always has an option of returning back to the original reactants. If it takes too long for the products to cool down, then there is a good chance that the product will revert back to its reactants, leading to no reaction. That is why understanding what factors affect this time is important.

Q. What methods are available to study this, and which do you work with?

One method is to heat up a molecule very precisely using lasers. Then we wait, and see how much energy the molecule has after a certain period of time. The molecules move really fast, on the timescale of femtoseconds which is a millionth of a billionth of a second. Ahmed Zewail developed a technique of 'pumping' energy into, and 'probing' the molecules on femtosecond timescales in 1980-1990, and received a noble prize for this work!

Another way, the approach I use, is to simulate this process on a computer. The molecule is modelled in some form – a simple way is to think about billiard balls connected through springs. The balls represent atoms and the springs represent chemical bonds. We can tune how stiff these springs are to model different kinds of bonds. We can even see how these springs will act in time based on methods proposed by Newton. Voila, now we can put energy in by stretching the bond, and see how it dissipates in time. Computers can be very efficient in simulating this.

Q. How do you know this computer modelling works? It seems a stretch of imagination to compare springs with bonds.

This is where the kind of experiments designed by Ahmed Zewail greatly helps. Fleming Crim, a professor at UW Madison, and his group performed a similar experiment on a molecule called chloroiodomethane. This molecule is important for environmental reasons. If our computer model agrees with the experiments, it gives us a great deal of confidence. This kind of computer modelling was started in 1965 by four scientists – Fermi, Pasta, Ulam and Tsingou, and has made great progress since then. In fact, last year's Nobel prize was given to Karplus, Levitt and Warshel for the developments they have done in these computer simulations. These simulations have been proven to simulate chemical reactions with some accuracy.

Q. But why perform these simulations if you can watch the real molecule itself?

Simulations contain far more information. You know the motion of every atom, and the details of the energy flow. Not only that, one can also change the stiffness of the bonds, or how much energy was initially put in and observe the change in the results. This gives us the ability to generalize and predict the time of energy flow in new molecules. These changes are very hard to do in the experiments.

Q. Briefly, what are the key results of this work?

The time of cooling I obtained roughly matches the time seen in the experiment. What I further obtained is the speed and pathways of energy flow – very rapid at the beginning, slowing down later. The slower time depends on how stiff the bonds are. The stiffer the bond, the slower the energy loss. Another crucial factor is the partitioning of the energy among the bonds after the rapid energy flow at the start. If the stiffer bonds retain

more energy, then the overall energy flow will be slower.

Q. How does your research affect society?

All applications originate from a better understanding of how nature works. Galileo's thorough study of celestial motion became the precursor to the Newtonian mechanics, which has a vast range of applications. My work adds to our understanding of tunneling and energy flow in molecules, both of which are relevant to society. For example, based on the methods presented in this thesis on tunneling, more simulations and better experiments can be designed to develop medicines to fight tumors. Similarly, with a better understanding of energy flow, we can control the flow of energy. In doing so, we can manipulate reactions to our advantage – for example we can use this research to improve solar cells by increasing the fraction of the sunlight energy that converts into chemical and electrical energy.