Interview Assessment 8

Date: October 28, 2021

Subject: Computational Chemistry

Source: Prof. Steven Nielsen

Assessment:

This interview with Dr. Nielsen provided unique insight into one area of computational chemistry: molecular dynamics (MD). This field uses computers to simulate the movement of atoms and molecules and has diverse applications throughout chemistry, engineering, and biology. Dr. Nielsen broke down his duties into three parts: research, teaching, and service. The former involves publishing papers and writing grants for computers for his lab. Teaching involves leading undergraduate and graduate courses, grading exam papers, and even supervising research for undergraduate students. I expected service to relate to outreach or volunteer work, but he said it primarily encompasses administrative work like serving on committees to hire faculty or admit grad students. However, Dr. Nielsen also included tasks like judging science fairs and overseeing student organizations at UTD. He mentioned that writing grants could take as long as you want, but it's a personal decision to limit the amount of time spent on work. Work-life balance is also important for students, according to him. As many chemistry students get burned out when they're also working, Dr. Nielsen believes it important to maintain hobbies—squash, for him.

Specialized fields like molecular dynamics can be difficult to understand at first, so I learned a lot from an example he shared. Dr. Nielsen once collaborated with mechanical engineers (his work is highly interdisciplinary and collaborative) on a project to capture water vapor efficiently in arid environments. He needed to identify the angle that water droplets make

with the surface, as this is a measure of how spherical the droplets are or how hydrophilic the surface is. Using a computer simulation, he could model some thousands of water molecules on the interface of this surface, but how would you identify the molecules that are on the surface of the droplet? The solution was establishing a fixed-size circle around each molecule and counting the number of atoms around it. Molecules in the air will have none, whereas those in the interior will have many. The molecules on the surface will have a count that's in between. From there, you can fit a curve and then calculate the angle. My big takeaway was the general process for approaching MD problems. Previously, I thought you attempted to solve an equation analytically and then approximated a solution numerically. Instead, I realized that the process is more about creating an algorithm on paper and implementing it with code. I also learned that research results are often field-specific: for an application relating to delivering neuropeptides in the brain, chemists would not consider the plethora of molecules in the blood. Instead, an expert in medicine would pick up the research and apply their domain knowledge to create a solution.

In terms of skills to have, Dr. Nielsen differed from other professors I have interviewed. He believes in focusing on developing a robust math and physics foundation since those subjects are difficult to self-study (and I wholeheartedly agree). Surprisingly to me, he said you can pick up the biochemistry that's necessary through reading. A strong foundation in chemistry is helpful for collaborating with other chemists, but it's certainly less important to him than to Dr. Tao, possibly because computational chemistry is computer-based. However, even coding does not warrant taking a class, according to Dr. Nielsen—rather, it's important to gain practical experience, which makes sense. He also hasn't yet expanded into using machine learning, which he says is the most important recent development, so a strong computer science background probably isn't as important. Naturally, his advice to me was to be proactive and learn what I

could right now, including coding and the latest developments (through Scientific American, if not a peer-reviewed journal). He believes conducting research is also a good idea for young scientists. I'm glad to have dipped my toes into that, and I'm looking forward to continuing my ISM work this year after having better understood the field from this interview.