

Mentoring Philosophy and Practices Statement

I was the first person from both my parents' families to receive high school, and higher education degrees, including BS, MS and Ph.D degrees. Although both my parents valued education, they felt they could not provide effective advice for my educational and career goals. This fact pushed me from an early age to seek advice from people outside my comfort zone. At the same time, I learned to value honest feedback, and I highly appreciated people who acted as my mentors in my career. As a result, becoming a professor at Pitt gave me the opportunity to do something that is close to my heart: mentor doctoral students. My passion for academia was instilled when I was engaged in an international collaboration in Germany being an undergraduate student in Greece. Thus, it became clear to me before graduate school that to solve important problems you need to work with many scientists across the world and collaborate effectively in multicultural and diverse environments. The best part of being a professor is to interact daily with young researchers, who are building their careers based on their dreams and aspirations. My mentoring approach is built around providing what is needed to see my doctoral students grow and achieve their career goals.

Mentoring style: Every student is different in terms of personality (e.g. extrovert vs. introvert, feeler vs. thinker, etc.), academic strengths and weaknesses, career goals, prior experiences and training. As a result, I closely observe my students and I adjust my mentoring style in a way to fulfill their needs and make them feel comfortable. I interact with all my students on a regular basis, through weekly group meetings, individual meetings, and pop-up meetings (where students just show up in my office or I stop by the lab to ask them how they are doing and if they need anything). I regularly take "mentoring walks" with them where we walk on campus and discuss their goals and strategies to accomplish them. My priority as a mentor is to always keep a strong culture of teamwork in my lab. I believe that being successful in your career involves working as part of a team and being supportive to your teammates. Importantly, I follow a "work hard, play hard" way of life and I highlight that no matter how hard we need to work to be successful, we should always dedicate time for us and our families and enjoy life outside the lab.

Focus on high impact problems and develop critical thinking: The research in my lab focuses on applying computational modeling to solve important problems for Energy and the Environment, areas that are facing unprecedented challenges nowadays. However, solving challenging scientific/engineering problems is not trivial and involves strong effort and, often, frustration. I always remind my students that behind every success story there are many stories of failure, and that every time we fail there is an opportunity to grow since we know what went wrong and how to improve. What is most important, especially in a PhD, is not the outcome but the path you followed to reach this goal. I use the elenctic method of Socrates to guide my students' thinking on how to approach a research problem and help them develop critical thinking. My favorite questions are "What do I learn from this? Why do we care?". I highlight how important it is to be able to evaluate the validity of their results and how their findings fit in their overall research projects.

Provide cutting-edge technical training: Solving challenging problems requires keeping high standards in the training of the next generation of scientists and engineers. At the same time, a mentor should explain how meeting these standards will help the student's career development. I challenge my students to get outside their comfort zone to learn new skills and grow as individuals. My mentoring starts before my students officially join my lab as soon as I am engaged in discussions as a potential advisor. My first question is if they aspire to join academia or industry and based on their response, I work strategically with them to successfully accomplish their goal. For example, students who desire to join academia focus more on fundamental research problems and are given ample opportunities to engage in teaching and outreach. On the other hand, students who desire to join industry focus more on applied problems and make connections with economic aspects and optimization of industrial processes. To this end, I provide my students interdisciplinary technical training involving Computational Chemistry, Multiscale Modeling, Data Science, Machine Learning and Scientific Computing, blending concepts from Chemical Engineering, Physics, Chemistry, Materials Science and Computer Science. Providing cutting-edge research training and mentorship to the next generation of scientists and engineers goes beyond my research group. My graduate courses are designed to develop and apply research skills that my lab provides. Thus, doctoral students from

different departments and research groups have collaborated with me transforming their course projects into publishable research studies. Importantly, I interact at national conferences with students from other Universities and I enjoy discussing common challenges in academia and how to address them. For this purpose, I have been invited by the University of Delaware, the Mississippi State University and Greek Universities to lead discussion panels with doctoral students about challenges in graduate school and how to address them.

Engage in multidisciplinary, international collaboration: To develop cutting-edge research skills and solve important problems we need to work together with the whole academic community. All my students work with other researchers at different levels, disciplines, and countries. For example, PhD students have opportunities to act as mentors working closely with undergraduate researchers, as well as collaborate with experienced researchers, such as postdocs and senior scientists (e.g. at National Labs). In addition, all my PhD students are involved in collaborative projects with experimental groups with complementary expertise in other Institutions, both Nationally (e.g. CMU, U. Rochester, U. Houston, National Labs, etc.) and Internationally (e.g. University of Oxford (UK), Chalmers University of Technology (Sweden), Politecnico di Milano (Italy), etc.). A recent example is my year-long sabbatical in the Department of Physics at Chalmers University in Sweden. I worked with four of my PhD students to attract funding from multiple sources to fully support their travels during my sabbatical, so they receive training on new computational methods, and experience research in Europe, a completely different work and cultural environment.

Communicate effectively: Central to performing collaborative and cutting-edge research is effective communication. Communication is a two-way process, involving presenting scientific results in an exciting, engaging, and effective way, as well as listening, interpreting, and addressing scientific questions. However, communication can be challenging between researchers at different levels and disciplines, as well as between researchers and the local community. As a result, I emphasize developing outstanding communication skills and learning new graphic tools to prepare eye-catching pictures and breathtaking videos. Effective communication also entails understanding your audience and adjusting your presentation to capture attention. For this purpose, my students present research talks and journal clubs in our group meetings, write reports and scientific manuscripts and participate in technical writing workshops. All my students individually receive detailed feedback on their presentations and written documents. As a result, several of my students have received best presentation and poster awards at National Conferences, whereas 21 scientific articles from students I advised at Pitt have been featured as journal covers.

Provide an environment of growth and success: It is very important for me as a mentor that my students feel valued, and they are provided the best opportunities. I encourage my students to attend computational training workshops and every year all my students present their research results to at least one national (e.g. American Institute of Chemical Engineers, American Chemical Society, etc.) and to one local conference (e.g. Pittsburgh-Cleveland Catalysis Society, Pittsburgh Quantum Institute, etc.), which I financially fully cover. I support my students in writing competitive National Science Foundation (NSF) graduate research fellowship (GRFP) applications. I have developed and delivered NSF-GRFP workshops for all the Swanson School of Engineering students with 45 Pitt students having received NSF-GRFP awards and 28 honorable mentions in the 5 years that I lead these workshops. Three of my PhD students (Austin, Taylor and Miu) have been awarded NSF fellowships after they joined my lab. I nominate my students for multiple awards, travel grants and prizes both at national and international levels. The best part of these awards is when the student is not aware of a nomination and suddenly receives a prestigious award! Examples include being selected as the best computational PhD researcher in the U.S. by the American Institute of Chemical Engineering (2 PhD students from my lab), as U.S. delegate to meet with Nobel Laureates in Lindau Germany, as conference travel grant awardees, as recipients of Braskem and Coull awards from Chemical Engineering (awarded to the best 2 PhD students in ChE every year – 5 out of 7 of my PhD graduates at Pitt have received these awards), etc. Moreover, I strategically utilize the conferences to create opportunities and motivate my doctoral students. I connect my senior students with potential employers both in industry and academia based on the network I have developed over the years, and I introduce my junior students to academic leaders in our field, so they feel that they are an integral part of our research community. I invite my graduate students to meet with our departmental invited speakers, so they receive different career

perspectives and advice. Finally, I communicate my students' accomplishments to the whole lab and their highly prestigious awards to our Department Chair and we publish news releases about their tremendous successes. I also organize regular group dinners/lunches to celebrate all the successful stories of each individual student in my lab.

Prepare students for future professional roles: One issue I have noticed in academia is that although Universities provide an environment to learn and grow technical skills, our students often fail to receive some general guidance on how to grow as professionals and what to expect in industrial and academic settings when they are asked to lead research groups. This issue is more pronounced when it comes to intellectual property. For this reason, prepare and deliver every year presentations to my group about good practices in a research lab, what to expect in interviews and how to handle job offers, how to deal with conflict and a series of hypothetical scenarios relevant to protecting intellectual property. These presentations have been proven extremely useful not only because they can help everyone with their career, but because they present real-life scenarios that the students may have never experienced before. Most recently, though my leadership, I formed a junior advisory board in our department with industrial and academic experts from different areas and one of their roles is to mentor our doctoral students to prepare competitive skills. In addition, I am leading the academic stream of a recent NSF award in our department, where I organize training workshops and prepare our doctoral students for future careers in academia.

Promote diversity and multicultural research environment: I have been very fortunate to be the mentor of students from underrepresented minority (URM) groups and from different gender, cultural, ethnic, and religious backgrounds. I am participating in the Pitt STRIVE program and I have served as an AGEP advisor to two URM students (one graduated and one current). I am thrilled to have worked with individuals from U.S., India, China, Italy, Pakistan, South Korea, Venezuela, Mexico, Kuwait, Egypt, etc., to solve important scientific problems. To establish such a diverse environment, I put a lot of effort on recruiting students at national and international conferences and meetings. For example, I attend undergraduate poster sessions at the AIChE national conference, and I meet with prospective graduate students, including URM, to discuss about their goals and how Pitt, and specifically my lab, can help accomplish them. This is what science is all about: bringing together outstanding researchers from diverse backgrounds with inclusion and equality to solve big problems.

Measure mentoring impact and improve: A question that is very difficult to address in academia, no matter the area of research, is how do you measure impact? This is even more challenging when it comes to doctoral mentoring. I personally measure impact through the success of my students. All my doctoral students have been highly productive in their PhDs and their research results are published in premier journals including Nature, Nature Communications, Science Advances, etc. As mentioned above, their success is reflected on the multiple prestigious awards they have received. All PhD students graduated from my lab have been extremely successful in academia, national labs, and industry. I can proudly say that all my PhD graduates were placed in their dream jobs and positions and had received multiple offers before graduating from Pitt. I keep in contact with all my past students since a mentor is for lifetime, and I enjoy hearing about all their successful stories. Despite my students' success, mentoring is dynamic. It can change over the years based on the member demographics of the group. As a result, an effective mentor needs to always be able to address the student's needs. For this reason, I have taken a series of team management and personal training workshops with Devora Zack, a best-selling author and leadership consultant on how to improve as a mentor. Some of these workshops were part of the Center for Faculty Excellence, while others were taken out of my personal interest. In many of these activities I engaged my graduate students to participate, so I further understand their personalities and receive feedback on my mentoring practices.

To conclude, the individual who is mostly benefiting from the mentoring process is the mentor. I enjoy seeing my students grow personally and professionally, develop technical skills and critical thinking, reaching their career goals and becoming highly successful in industry and academia. Most importantly, I love being educated by my mentees, attacking new problems with methods and techniques that I had never thought about before joining Pitt. My journey as a mentor has been very exciting and rewarding!