

# Judy Marouf & Anastasia Duenas | *Bytes and Bonds* Podcast, Spring '23

## Summary of topic

For our podcast project, we chose to explore the topic of computational chemistry and its role in modern chemistry. Computational chemistry is a field that uses computer algorithms and simulations to study chemical systems and processes. As the complexity of chemical systems has grown beyond the capabilities of traditional experimental methods over the decades, computational methods and tools in chemistry have become increasingly important.

In the first episode of the podcast, we shared some background information on how we reached the topic of our podcast before jumping into an overview of the role of computational chemistry in modern chemistry and the importance of computer science in the field. We discussed how computational chemistry has become an essential tool for understanding chemical reactions and predicting the properties of molecules and materials. We also highlighted some of the key advantages of using computational methods. In our second episode, we introduced the discussion by covering the history of computational chemistry. Specifically, we shared the work of John Pople, a British theoretical chemist who laid the foundation for many of the methods still used today in computational chemistry. We demonstrated how Pople's groundbreaking work revolutionized the field of computational chemistry and made it possible to accurately model the electronic structures and properties of molecules. In the final part of the episode, we detailed some of the latest computational tools being developed by researchers to predict the properties of molecules and materials. We outlined the growing use of Machine Learning and Artificial Intelligence in computational chemistry and how these technologies are changing the way chemists approach problems in the field. Finally, we presented some of the key benefits and limitations of using these tools.

## Approach

Considering the vast technical topics in STEM out there that we could have delved into, we decided to approach the project by figuring out a way to merge both of our programs of study and interests into one. We did this by taking computer science (Judy's major) and chemistry (Anastasia's major) and researching the various ways in which these fields intersect. Eventually, we narrowed it down to the growing field of computational chemistry. In doing so, we were both able to speak about this topic with passion and proficient background knowledge—all while having fun and enjoying every step of our progress. We found that this topic had great potential in terms of the various areas we could cover about it, including things like its overview and history, but also the several computational methods and their applications, and the modern-day computational tools being developed by researchers. Throughout the podcast, we made sure to apply our perspectives and thought processes to create a more personalized touch to our series.

## Experience & Growth

Making a podcast was a new and genuinely rewarding experience for both of us. We learned so much along the way and progressed our research skills while preparing for each episode—a process which involved reading articles, watching videos, and conducting interviews with experts in the field. We learned how to effectively structure each episode in a way that would be engaging and informative for our listeners. We grew in our ability to work as a team, to communicate effectively, and to adjust to any unexpected setbacks. We learned to support each other's strengths and weaknesses, and we developed a greater appreciation for the value of collaboration. Overall, making this podcast was a challenging but valuable experience that allowed us to enhance our current skills and develop new skills to grow on a personal and professional level.