Tell us about your work with computational simulations and green energy or fuels - do you have an analogy or layperson’s way of describing your work?

We are currently interested in harnessing and processing carbon dioxide in our atmosphere to create green energy solutions. If we combine carbon dioxide and hydrogen, we can create methanol which is currently used as a fuel. Our research focuses on theoretically simulating catalysts, such as copper, reacting to carbon dioxide to create methanol. Computational simulation, my area of expertise, assists in keeping testing and experimentation costs low so we can continue to investigate until we find a suitable reaction.

Why or how is your area of research and discovery important for ordinary citizens?

Our research is dedicated to finding alternative, renewable fuel and fuel cells. Using methanol as an easy-to-transport anode and oxygen as a cathode, the reaction creates energy. This energy is converted to electric power, but the products of the reaction – carbon dioxide and hydrogen – may be reused to generate more fuel. We are taking something which is harmful to our environment and creating a useful product that can power our cars or (one day) buildings. There are many applications for this research.

What is your favourite aspect of your research? What is most exciting for you?

Working with computer simulations allows us to predict the materials and methods that would be most suitable for our work, while avoiding the heavy cost in time and resources. Computers create an efficient testing environment; when the right materials or processes are found, the experiment can be physically conducted, helping us skip the lengthy trial-and-error process. Experimentation can take a long time and it provides one part of the picture. The performance of computers becomes 10 times approximately in every 4 years - we can get more done as our computers become more and more efficient - and we are able to conduct experiments at a microscopic level. Simulations provide a fuller idea of what is taking place.

Is there an area in your field (or outside of your field) that you would like to explore in future?

I would be interested to simulate chemical reactions in biological systems or humans - there is still so much we do not know about our brains.

Do you have any advice or words of wisdom for our students?

Find your interest!