

Portrait of recipient of Elite Researcher travel scholarship 2022

Name

Andreas Erbs Hillers-Bendtsen

Job and titles

ph.d.-student, Msc in Chemistry

Birthyear

1996

Research Area

Physical and Theoretical Chemistry

Project Title

Exploring Molecular Systems for Exploitation of Solar Energy & Development of Cluster Perturbation Theory

Brief project description

My ph.d. project concerns design and discovery of new molecular systems for exploitation of solar energy. A central theme is to discover new and better molecules for the molecular solar thermal energy storage technology which exploits the ability of some molecules to undergo reversible chemical reactions following the absorption of sunlight. Using this concept, these systems can potentially store thermal energy in chemical bonds. The stored energy can later be released as heat in a closed system without the emission of CO₂ or other greenhouse gasses. I am figuratively speaking trying to find a needle in a haystack that is exactly the molecules that would be best suited for this technology. For my work, I utilize and develop different quantum chemical methods in order to simulate the properties of new molecules and use the results to rationalize whether our candidates are potentially better than existing technology. Based on my predictions, our experimental collaborators abroad try to synthesize these molecules and test them for solar energy storage.

How I became interested in my field of research

During the first two years of my bachelor studies in Chemistry at the University of Copenhagen, I became very interested in quantum chemistry. I found it deeply interesting how quantum mechanics can be used in combination with other theories to actively predict the properties of molecules, the outcomes of their reactions, and their interaction with their surroundings. Furthermore, the ongoing climate changes in the world concerns me and I therefore find extra motivation for applying theoretical chemistry to explore and design molecules and technologies that can possibly aid the transition towards sustainable energy production.

What are the challenges in your research project?

There are many challenges in my project. One challenge is that there exists an infinite number of different molecules, at least theoretically. This means that even with the massive supercomputers available today it will be impossible for us to investigate all of them for exploitation of solar energy. We are therefore actively working on establishing more knowledge on what characterises

molecules that are good at storing solar energy and how we can optimize existing molecular systems. A second challenge is to develop theories that can accurately predict molecular properties and to implement them efficiently in computer software that can exploit the computational resources of large supercomputers. Presently, we have methods that can very precisely predict molecular properties, yet, these simulations take a very long time to run even with the supercomputers of today. It is thus a large challenge in the field of theoretical chemistry to overcome this problem and my project also deals with this.

What does the Elite Researcher travel grant mean for your research project?

The Elite Researcher travel grant will support my stay at Stanford University in USA during 2022-23, where I will visit one of the world leading research groups in the field of modelling photochemical and photophysical processes which are essential for exploitation of solar energy. My visit will seek to expand my knowledge on these methods both theoretically as well in terms of programming them, as they also specialise in using graphics cards for accelerating quantum chemical calculations at Stanford University. Finally, it is also a great opportunity to strengthen my network internationally and thereby strengthen my future career within research.

Something on the person behind the researcher

I was born and raised in Jutland, more specifically in Aarhus and Skanderborg. After high school, I moved to Copenhagen to study Chemistry. Nowadays, most of my time is spent on research for my ph.d. project, but in my free time I often go for long walks, running, or biking together with family and friends. In addition to that, I am very interested in sports and have been playing badminton for many years. I therefore also spent a lot of time watching soccer, basketball, etc.

Contact info

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Research institution

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