Prof. Veronique Van Speybroeck (CMM – Center for Molecular Modeling, Ghent University) is recipient of the second MCEC Lectureship Award. In September 2018, she visited the different MCEC research groups, gave scientific lectures and participated in scientific discussions. Daan from the MCEC Office exchanged many e-mails with Veronique in which she reviewed the current state of the research field of molecular modeling as well as articulated three Grand Challenges for the future.

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Interview with Prof. Veronique Van Speybroeck

During your MCEC lectureship, you brought members of your group to Utrecht to engage in a symposium around three Grand Challenges. Can you tell a little more about these grand challenges and why you chose these?

As I prepared my visit and my lectures together with a core team of my researchers, we took the opportunity to brainstorm about the status of our modeling approaches in the field of nanoporous materials. With the framework of my ERC Consolidator grant, we have invested a lot of effort to model at operating conditions, thus taking into account realistic conditions of pressure, temperature and guest loadings in the materials. However, to model some processes and reactions even more accurately, it is essential to develop new methods and techniques.

The brainstorm session allowed to clearly identify some major challenges for the future. One question is how to deal with imperfect materials or with various domains in the materials with different properties. Today we are still modeling fairly small systems of the order of a few nanometers. However, to understand processes such as amorphization of materials or collective phase transformations, we need to develop models that extend the length scale to the order of the crystal size. We are now taking our first steps in this direction.

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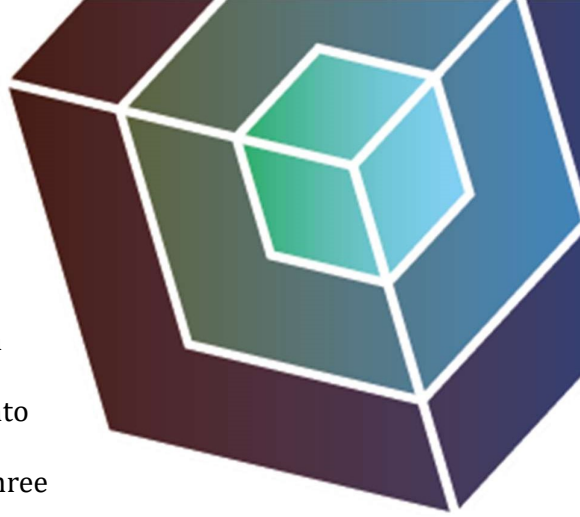
Another challenge is related to the history of the material and the process. We all know that materials behave differently depending on their pretreatment or the number of reaction cycles that have taken place. In many cases we do not take these aspects properly into account. In this sense, we believe we need to also develop models which cover the lifetime of the materials and processes.



I think it is very important to always question the methods and approaches you use, to identify the next big steps you would have to take. As we are doing almost all our modeling work together with experimentalists, and knowing many problems are inspired by real experimental problems, we get a good feeling of which phenomena we are able to describe with our current methods and which effects we are not yet taking into account properly. The synergy between theoreticians and experimentalists is also an essential driver in pursuing these three challenges.

What important new insight has your Lectureship yielded?
In molecular modeling we typically use a bottom-up approach, where we start from the atomic scale and try to mimic realistic conditions and systems as well as possible. Spectroscopy typically uses a top-down approach starting by looking at the materials from the outside and trying to resolve as much detail as possible. Both fields have evolved substantially in the last decade and we are now entering the era in which spectroscopy and modeling are starting to meet each other.

With the help of spectroscopy, we can distinguish phenomena with a resolution that enables us to put forward hypotheses about e.g. reaction mechanisms and active sites at the atomic scale, which are typically validated by modelers. From the interactions we had with the people in Utrecht, several common research questions were defined, such as how to follow phase transformations of flexible materials, how to identify reaction intermediates or how to characterise diffusion paths of molecules. So it was really inspiring to have intensive discussions with a group of people working in spectroscopy.

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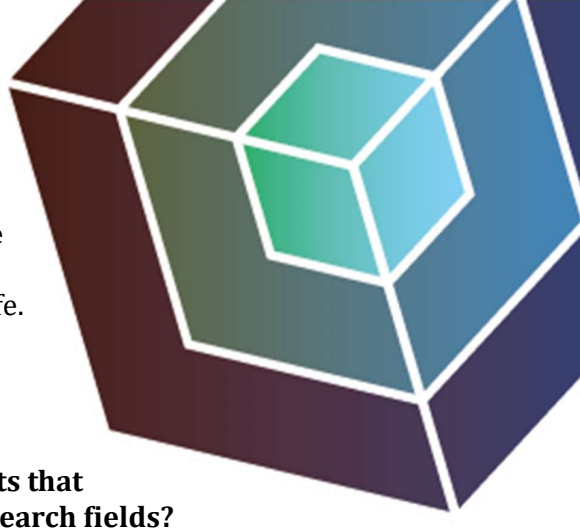
How would you describe the MCEC Community?
I was very impressed by the MCEC Community, as you cover a real broad area of disciplines and research topics. I strongly believe that such an interdisciplinary collaboration is essential towards solving major challenges we are facing in our society, for instance related to sustainable energy supply and conversion, clean air, water supply… It is a visionary approach to set up such communities between people from really different disciplines for a longer period.

It typically requires a longer time to see the fruitful effects of such collaborative communities. From my own experience, I know that it usually takes more time to collaborate with people with different backgrounds. The first challenge is always to understand each other's scientific language. Once you reach that point, researchers can start to tackle common research goals. Therefore, it is truly necessary to install such collaborative efforts for longer periods and with enough critical mass to really make the difference, as is perfectly illustrated by the MCEC Community.



I was also impressed by the highly motivated PhD students and researchers. I had the feeling they were all very passionate about their research. I am always very impressed to see such passionate young people starting to build something in their life. To be able to coach and guide young people along their path, is probably one of the most beautiful aspects of our role in academia.

After 18 years of CMM, what would you advise PhD students that are new to working with different concepts from other research fields?
To embrace new ideas and challenges, to strive for fruitful collaborations and look beyond their own specific discipline. New PhD students should be able to receive maximum freedom to explore new ideas. They should be able to bounce off these ideas with their advisors and other people in their environment.

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You are co-founder of the Center for Molecular Modeling in Ghent. What is the biggest challenge in leading a multidisciplinary research team such as this?
To maintain this idea of collaboration between all members in a continuously growing research group. Among all these years we were able to attract the top students to our group with all kinds of backgrounds. Each of them is very good in their own discipline but the key towards excellence is working together, sharing and building on each other's ideas.

How do you deal with this challenge?
I try to maintain a very open communication culture, as we are all researchers with our own strengths and weaknesses. I very much realize that we are stronger together. I try to create a fruitful intellectual environment, without boundaries. When we tackle a scientific question and feel the need to involve someone with a complementary expertise, we always do so. As we have people with many different backgrounds, such as physicists, chemists, and engineers, this often leads to very innovative insights. In this process, all the researchers need to be valued. Everybody needs to get the chance to present their results, to be strongly involved in work discussions, and so on.

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Apart from the professional activities, we organise social events on a regular basis. Next to the science, it is very important that people feel at home at the research center. Even little things – like fresh fruit in the kitchen every week or installing the Christmas tree together – help in this social bonding. In that sense, I was also very happy that we could organise a mini-conference during the MCEC Lectureship in Utrecht where various CMM researchers could interact with the researchers at the Debye Institute. It underscored the feeling that we are in this adventure together.

How did the Center for Molecular Modeling come into being?

I started my research in molecular modeling in the late nineties under supervision of Prof. Waroquier who was a theoretical physicist in Nuclear Physics. He wanted to start a new research direction by extending various theoretical many-body techniques applicable for nuclear systems to molecular systems. I was involved from the start in the launch of the new research field.

During my master, I already went to a Summerschool in Cambridge organised by Prof. Handy, an authority in Density Functional Theory (DFT). Furthermore, around that time, DFT was flourishing within the field of molecular modeling. In 1998 the Nobel prize in Chemistry was awarded to Walter Kohn and John Pople for their developments in Density Functional Theory and computational methods in quantum chemistry.

I was trained as an engineer in Physics but from the onset I was very much intrigued by the application of theoretical methods to "real" applications, also with industrial relevance. I think that was also the reason why after obtaining my master thesis, I undertook a research visit to DSM Research in the Netherlands under supervision of Dr. Robert Meier and Dr. Solange Blaszkowski. This experience was very instructive and I was very much intrigued by the application of molecular modeling techniques to industrial applications.

"From a managerial point of view, such an approach is not the easiest but it is precisely this multidisciplinary approach which is the key towards excellence."

At Ghent University, there was no research group in molecular modeling at that time. From the onset we started by making strong connections with chemically oriented groups. We wrote projects to obtain funding for the new research line and attracted good students to the new group. It was immediately clear that we could make a difference in the world of molecular modeling thanks to our physics background and our connections with experimental chemistry and engineering groups.

The DNA of the CMM – founded on the idea of bringing together physics, chemistry, engineering… and strong collaborations between departments of the faculties of science and engineering – was born in these initial days.

Today, we are still a multidisciplinary center with PIs from various faculties and departments and we span the broad field from fundamental to application-oriented research. Our multidisciplinary center is very unique also within the university as we group researchers from various departments based on their ability to contribute to our research goals. From a managerial point of view, such an approach is not the easiest but it is precisely this multidisciplinary approach which is the key towards excellence.