



Roderigh Rohling

Theory of Lewis Acid Zeolite Catalysis for the Conversion of Biomass-Derived Furanics – *on the Effect of Multi-Site Cooperativity and Confinement*

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23 January 2019

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“I am intrigued by the newly emerged CRISPR-CAS method for genome editing. Despite having thought about it numerous times already, I am still not sure how to position this method ethically; we should evaluate this method and its applicability very carefully.” – *Roderigh Rohling*

What was your dissertation about?

I performed a computational study (periodic DFT) taking the chemical complexity of the actual alkali-exchanged faujasite catalyst into account as opposed to the conventional modelling efforts using highly reduced models. I used the improved models to study the Diels-Alder Cycloaddition/Dehydration reaction between biomass-derived furanics and ethylene towards drop-in aromatics. The increased chemical representation makes interpretation of the results more difficult, but yields better descriptive and predictive power.

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I show that the collaboration between active sites and the spatial constraints they impose on the reactants are key factors governing the reactivity of zeolite catalysts. Furthermore, conventional Diels-Alder Cycloaddition theory based on isolated site and substituent considerations do not hold in these catalysts anymore.

What result from your research are you most proud of?

Most of all my dissertation. Not necessarily because I finished it (which is of course nice!), but especially because it is one smooth storyline resulting in one coherent piece of work.

A close second is my first 'first author' publication [[ACS Catal., 8 \(2018\) 760–769](#)]. Not because it is my first 'first author' publication, but because we coupled periodic DFT calculations to microkinetic modelling with experimental verification of the theoretical predictions. In my view a nice bottom-up approach combining different length- and time-scales.

What will you miss most about working at MCEC?

Bubbles! To me, this word is undoubtedly correlated to MCEC. But, aside from this (semi-) joke, I enjoyed the sessions and deliberations with colleagues from the different fields in science. It was great fun to get to know the MCEC members and to get acquainted with their work throughout the years. I think we really became a community and I regret that we all have to go our separate ways eventually. It was great to be able to contribute to the MCEC-Outreach activities via (invited) lectures for high school students.

I still remember the discussion I had with a bubble-scientist for about 30 minutes concerning mass transfer from the liquid phase to a bubble on the surface. We did not understand each other as we were using different terminology. Eventually, we discovered that we were talking about exactly the same thing at the moment we finally drew a schematic picture! A useful lesson for my future career.

At the start of your PhD, you mentioned you loved the field of zeolite catalysis. Is that still the case?

Zeolites are still very fascinating to me. I have developed a personal view on the characteristics of these materials now (properties, dynamics and catalysis). I find it fun to work with these materials of which we still do not know how nature creates them, yet we can do so many useful things with them.

In addition, I started to become intrigued by the newly emerged CRISPR-CAS method for genome editing. Despite having thought about it numerous times already, I am still not sure how to position this method ethically; we should evaluate this method and its applicability very carefully. Nevertheless, I find it fascinating from a fundamental scientific point of view.

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What are your plans for the near (and distant) future?

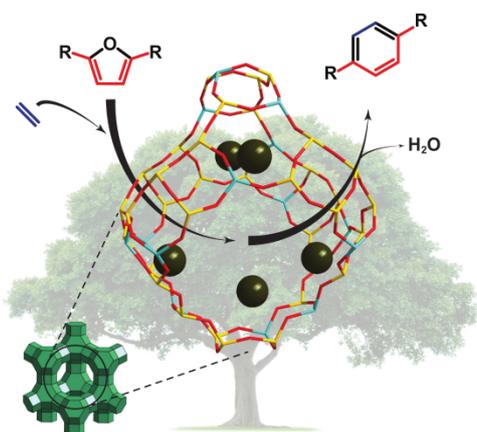
I really enjoy an academic position: doing research, writing articles, educational tasks (I really enjoy those!), attending conferences and giving lectures. However, I observed that many academic positions come with great uncertainty.

Thus, I prefer finding a (possibility to get a) long-term position somewhere, most likely industry. I will find more peace in my mind when I can develop my career and my personal skills without having to be concerned about where I will go and live next year.

To read the full thesis, click on the image.

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On the Effect of Multi-Site Cooperativity and Confinement



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