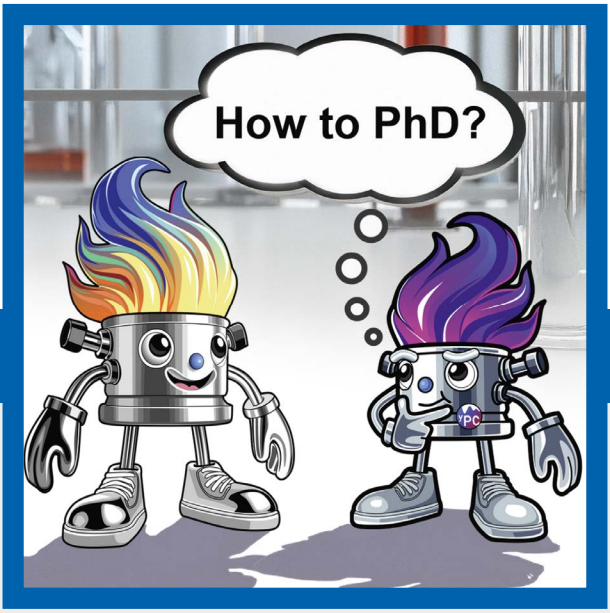
1/2025

BBPCAX 101 (8) 1083-1196 (1998)
ISSN 1611 – 9479

Bunsen-Magazin

Zeitschrift der Deutschen Bunsen-Gesellschaft für physikalische Chemie



Haben wir bereits Ihre E-Mail-Adresse?

Wir möchten klimafreundlich arbeiten und Sie gerne auf dem neuesten Stand halten und Ihnen aktuelle Informationen und Neuigkeiten zur **physikalischen Chemie und aus der DBG** liefern.

Dafür brauchen wir Ihre E-Mail-Adresse!

Und so funktioniert's:

Schreiben Sie uns eine Mail an geschaeftsstelle@bunsen.de oder gehen Sie auf www.bunsen.de unter *Login* und geben Sie Ihre Mitgliedsnummer und Passwort an. Unter *Meine Mitgliedsdaten* tragen Sie Ihre E-Mail-Adresse ein.

Kennen Sie den DBG-Stellenmarkt?

Nutzen Sie für Ihre Stellenausschreibung bunsen.de oder das Bunsen-Magazin

Ihre Vorteile sind:
- Gezielte Ansprache von Fachkräften aus der Physikalischen Chemie
- Kostenfreier Online-Stellenmarkt für Promotionen, Postdocs und Nachwuchsgruppenleitungen

Preise und Formate finden Sie auf www.bunsen.de/stellenmarkt

Sprechen Sie uns gerne an – Sie erreichen uns unter geschaeftsstelle@bunsen.de oder 069 7917-363

IMPRESSUM

Bunsen-Magazin

Heft 1 Jahrgang 27

Herausgeber:
Vorstand der Deutschen
Bunsen-Gesellschaft
Robert Franke
Ralf Ludwig
Ulrich Ott

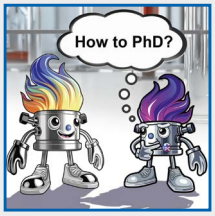
Schriftleitung Gasteditoren:

Noah Al-Shamery	noahcoel001@e.ntu.edu.sg
Tobias Dickbreder	tobias.dickbreder@univie.ac.at
Katharina Meyer	katharina.meyer@outlook.de
Arman Nejad	arman.nejad@chem.ox.ac.uk
Florian Schneider	fschneider8@uni-bielefeld.de

Geschäftsführerin der Deutschen
Bunsen-Gesellschaft
Elisabeth Kapatsina
Varrentrappstr. 40-42
D-60486 Frankfurt
Tel.: 069 / 79 17 363
Fax: 069 / 79 17 1363
E-Mail: geschaeftsstelle@bunsen.de

Technische Herstellung:
die printzen GmbH
Gewerbepark 21
D-92289 Ursensollen
Tel.: +49 9628 / 924 89-0
Fax: +49 9628 / 924 89-10
E-Mail: info@dieprintzen.de

Das Bunsen-Magazin
wurde auf recyceltem
Papier gedruckt.



Zum Titelbild:
A PhD is a unique and challenging journey for every young scientist, especially in physical chemistry or related fields. It can be complex, but mentorship from experienced scientists can help students decide if a PhD is the right path and what to consider when choosing a position. In this Bunsen-Magazin issue, yPC explore key options for tackling the question: "How to PhD?" Cover image: Simon Sprengel.

Katharina Meyer, Noah Al-Shamery

From Undergrad to a PhD or an Industry Position: Deciding the Next Steps After Your University Degree

Katharina Meyer

Noah Al-Shamery

Every chemistry student will eventually ask themselves what to do after finishing their bachelor's or master's degree. A popular choice after the latter is to pursue a PhD. But is a PhD even the right choice for me and my career ambitions, or am I doing it because everyone else is? Even if I am sure that I want to continue academic research, what research do I want to do and where do I want to do it? Many of these questions are difficult to answer and think about if you don't even know what is out there. This is why we, as the *young Physical Chemists* (yPC), have dedicated this issue of the Bunsen-Magazin to provide some insight to those questions.

These kinds of questions are very familiar to us, as we were both facing similar decisions in the past. Noah has decided to pursue a joint PhD abroad – partly at Nanyang Technological University Singapore and partly at the University of Warwick. A joint PhD comes with its own challenges, for example adapting to those new cultural and working environments as well as constant travel, but also many benefits such as being exposed to different ideas and techniques. Katharina, on the other hand, has decided to strengthen her knowledge of vibrational spectroscopy by pursuing her PhD in the same research group that she did her master's thesis in, moved to the United States to carry out postdoctoral research at the University of Wisconsin-Madison sponsored by a Walter-Benjamin fellowship, and shifted to industry after her postdoc where she now works in research and development and is able to apply many of the skills that she has acquired during her PhD and postdoc. Just like ours, there are many different career paths for physical chemists and the right choice is different for everyone. To help you get a better idea of what to look for and make the right choice for yourself, we sought advice from experts with different viewpoints to share with you in this issue of the Bunsen-Magazin.

This issue is divided into two parts – the first part focuses on the transition from a university degree to industry, a PhD, or even both – an industry PhD. Dr. Rob Bowles, a career and professional development adviser at the Royal Society of Chemistry, explains whether a PhD was the right choice for him and whether he would recommend it for you. Dr. Julia Koppmann, who works for the Career Service at the Bielefeld University, details whether the doctorate is an asset for your employability outside of academia. Dr. Johannes Dobbelaar, Vice President Global Technology Dispersions, Resins and Additives at BASF SE, discusses career opportunities for chemists in industry. Dr. Uwe Nickel, former chair of the DBG and partner at Proventis Partner AG, gives us his perspective on carrying out a PhD in industry, which is complemented by Dr. Lisa Büker's report of her PhD experience in industry. For those who consider an academic PhD, Prof. Dr. Berthold Kersting and Christian Zocher share with us the advantages of carrying out a PhD as part of an SFB.

Once you have made the choice whether or not to pursue a PhD, how do you make the most of it and how do you manage difficult situations you will encounter during your PhD? How do you adjust to a new working environment, which might be abroad? These and similar questions will be answered by former IUPAC president Prof. Javier García-Martínez, current chair of the DBG Prof. Dr. Ralf Ludwig, Charlotte Gerischer from Team Chancengleichheit of the German Young Chemistry Forum, and many others.

The second part of this issue is dedicated to research by early career scientists. These include, amongst others, Prof. Dr. Maren Podewitz, assistant professor at TU Wien, who explores the functionality of catalysts and how to improve them. Specifically, she models transition-metal catalysts with multiscale models which employ statistical and machine learning techniques. As an expert in photochemistry, Jun.-Prof. Dr. Julia Westermayr from Leipzig University details in her contribution how to understand and control light-induced processes by using machine learning techniques. Both also share their journey of finding their research topic and give great advice for young students wanting to continue academic research. Dr. Stefan Gugler reports on artificial intelligence inspired by Physical Chemistry for catalyst design and we introduce the research of the four finalists of the Agnes-Pockels-PhD award 2025. All four finalists will give a talk at the Bunsen-Tagung 2025 in Leipzig, where the award winner will be chosen. In this issue, we also have two contributions to "*your Publications: Communicated!*", which is a new segment highlighting papers by young researchers.

We are excited to share this issue of the Bunsen-Magazin with you, as we hope it includes valuable insights for any young researcher looking for advice on how to proceed with their career. The *German Bunsen Society* is a great place to build a strong network and learn about exciting new techniques and research in physical chemistry and we as the *young Physical Chemists* try to facilitate exchange between more established and early career researchers as well as industry representatives, to help you with any career question that you might have. We hope to see you at the next Bunsen-Tagung in Leipzig to continue these conversations!

Dr. Katharina Meyer, Noah Al-Shamery
Speakers of the young Physical Chemists (yPC)
ypc@go.bunsen.de

BUNSEN-MAGAZIN · 27. JAHRGANG · 1/2025

Robert Bowles

Was a PhD the Right Choice for Me and Is It Right for You?

I didn't set out to be a careers adviser, but I did want to be a scientist. I loved the uses and applications of science. My first degree was in applied microbiology and biotechnology and this led me to a PhD in which I sought to optimise the production of omega-3 fatty acids from marine microorganisms. This used a lot of analytical chemistry such as GC/MS and was my first real foray into chemistry. I did my PhD at the same university I did my undergraduate degree and on the day of my degree graduation a lecturer asked me what I was going to do next? I told him I had been offered a PhD in the department. Thirty years later I can still remember his response. "That's great! You can do anything with a PhD!". At the time I had no frame of reference to understand the power of these words, or a PhD, but now I do. In fact it's a crucial aspect of my job.

I work for the Royal Society of Chemistry (RSC) as a careers and professional development adviser. We have members all around the world in a wide range of jobs and sectors, academic and non-academic alike and I get to help them make decisions about their careers every day. I help a lot of people considering whether to do a PhD, those who have started one and are not sure whether to finish or not, those who are coming to the end of their PhD and are seeking their first job, or those who, like me, completed it many years ago. Having completed a PhD, and an industrially sponsored post-doc, provides me with deeper understanding into the process of gaining a PhD and its impact on your career.

A PhD was a good option for me. It unlocked a range of roles, helped me to secure a job at the RSC and 18 years later, I am still here. It has given me a range of skills I still use to this day. The ability to plan, problem solve and use data for decision making to name a few. And that's on top of my technical skills, which granted have got a little rusty (I haven't been in a lab for over 20 years). While I don't use my practical skills anymore, understanding „the language of science" and having a technical background is hugely important to me in my role where I have to relate to, and understand the career paths of chemical scientists. I can help them to communicate their work and their science to non-scientists, an essential skill when helping them to write a CV or apply for a job

Dr. Robert Bowles MRSC
Careers and Professional Development Adviser
Royal Society of Chemistry
careers@rsc.org
www.rsc.org/careers

So a PhD was right for me, but is a PhD right for you?

Well do one if:

- It'll be good for your career. No one expects you to have your whole career plan mapped out when you start a PhD, but having some ideas of where you want to get to can be useful. Be aware though that you may not get the career benefits of a PhD straight away.
- You do it with a purpose, because you want to and know why you want to do it and have a clear idea of what it could lead to. Consider how doing a PhD is going to help you achieve what you want in your future career.
- You want to be an expert in a particular area of your subject. If you complete a PhD you will be.
- You want to achieve something. You want to work hard and demonstrate a passion for your subject and show how much time and effort you put in and how motivated you are.

Don't do one because:

- A lecturer asked you to do one with them. If you wanted to do one and it's in an area that interests you then great, go for it. If you hadn't thought about doing one before they asked, and you're not sure why you want to do one, make sure you work that out before saying yes to them.
- You don't know what else to do. Doing a PhD can just seem like the next step on your path. You get to stay in an academic environment you understand. Make sure that you explore other career options and whether they appeal before you commit to a PhD. Doing a PhD is a huge commitment, so before you take one on, make sure you understand why.
- Your family, or others expect it of you, or because your family/friends are doing one, or have done one. Make it your decision, not someone else's.
- You think that just having a PhD will lead to a „management" or „leadership" role. It won't, unless you can demonstrate you have developed those skills during your PhD or afterwards, and even then the employer might want to see that backed up with relevant industry experience.

If you're thinking of doing a PhD there are 4Ps you need to consider
The Project – what will you be researching? Why does it interest and motivate you?
The People – who will you be working with? Your supervisor, research group and any collaborators
The Place – where will you be doing it? The department, university, maybe even the country you want to do it in
Payment – who's paying for it? Your fees, stipend and living costs.

Zurück zum Inhaltsverzeichnis

If you did a final year research project during your degree did you enjoy it? Could you see yourself doing research like that for three to four years? Doing a PhD isn't about how clever you are, but how resilient you are. Can you stick with it when you're two years in and still haven't got any meaningful data?

Do your research

Identify universities you might want to work at. Which research groups and departments align with your research interests? If they don't, it will reduce your chances for success. If they do, be prepared to show this in an application. Speak to your likely supervisor before you apply. You can use the conversation to get them excited about you as a candidate so that they are on the lookout for your application.

Skills you get from a PhD

To identify the skills you have developed from your PhD you need to think about yourself differently. Academic researchers learn to focus on their research and the output from it, measured by research papers published. Researchers master a huge range of techniques and can use a vast array of technical, specialist equipment and often regurgitate these on lists on their CVs. Including each technique „just in case". Most employers aren't interested in how long these lists are and have little interest in the technicalities of your research. Instead they'll teach you about the technical aspects of their product or technology once you're in post but they'll expect you to be able to pick them up quickly. They also want you to have a PhD for the other, non-technical skills you have gained during your PhD. These are skills you can transfer from your research to other sectors - hence their name, „transferable skills". You probably take these skills for granted and use them without naming them. They include skills such as your ability to manage a research project, communicate, analyse data and use it to find solutions to problems.

Let's look at a few of these skills in more detail to recognise the ones you have and how to describe them to future employers.

Project Management
This involves managing a project or projects from beginning to end. You have done this if you have completed a PhD or a post-doc role successfully. Splitting it down further, you have learnt how to identify goals and/or tasks to be accomplished and a realistic timeline for completion. You might have had to prioritize tasks while anticipating potential problems and will almost certainly had to maintain flexibility in the face of changing circumstances. Consider describing your PhD as an exercise in project management

Communication skills
These involve oral and written communication. As an academic researcher you'll be good at both. You'll have prepared concise and logically-written materials and communicated ideas in oral presentations to small and large groups in a research meeting, or presenting a poster or talk at a conference. You'll be used to debating issues in a collegial manner and participating in group discussions, using logical arguments to persuade others and or explain complex or difficult concepts in basic terms and language (teaching or training experience). A crucial point to note here is that presentation skills aren't the same as communication skills!

Using data
Every PhD generates a huge amount of data. In addition to data you also use information from a huge amount of different sources to shape your hypotheses or identify the next steps in your project, another valuable skill that many employers value.

Problem solving and innovating
If you've had an experiment not work or a piece of equipment fail and you had to work out why, or had to work out a new way of doing something then you have great problem solving and innovating skills. You've probably never considered what you do in that way. You just have to fix things to continue your project, but explaining it like that to an employer can show them you have these skills.

Am I too far into may career to start one now?

Just because you didn't do a PhD straight after your first degree, doesn't mean you can't do one now. I've worked with people who are retired in their 60's starting a PhD. People considering doing one mid career is not that unusual. Often they are just seeking „permission" to do one and I help them to decide if it's right for them. Supervisors often like mid-career PhD students as they are better motivated to complete and have clearly thought about why they want to complete one.

Whatever career stage you are at, a PhD is worth considering. It gives you a widely recognised and valued qualification, demonstrates a high level of technical expertise and lets you build a fantastic set of skills that are highly prized by employers, whether you are staying in the lab.... or not!

Dr. Robert Bowles

After an early research career in marine biotechnology, Robert moved out of the lab, gaining five years' experience in sales and marketing of educational software to schools. He joined the Royal Society of Chemistry eighteen years ago, and has managed a program of their successful education and careers projects. He recently provided careers input into the new RSC Pathfinder CPD planning and recording tool for members launched in Jan 2023.
https://pathfinder.rsc.org
As a qualified careers adviser, he currently works in the Royal Society of Chemistry's Career Management team, offering careers advice to their membership and the wider chemistry community.

BUNSEN-MAGAZIN · 27. JAHRGANG · 1/2025

Julia Koppmann

Is the Doctorate an Asset for My Employabilty Outside of Academia?

You have dedicated many years to achieving a master's degree in physical chemistry. Are you passionate about applying your skill set during your PhD studies now? Currently, about 85% of chemistry and 61% of physics master's graduates complete their studies with a doctorate. [1] If you decide to do so as well, you will be in good company. Often, the completely legitimate decision not to pursue a PhD even feels like an opt-out. However, if you are already glancing at job offers outside of academia, you will find that there is hardly any demand for a PhD besides the "usual suspects". Should you pursue a doctorate even if you are ultimately aiming for a career in industry? Let us have a closer look and turn a yes or no into a how.

Table 1: The UniWiND Competency cluster with selected sub competencies [2]

Expert competencies Continual extension and adequate application of subject knowledge Methodological competence Familiarity with one's own community	**Systematic working** Collection and management of information Analytical thinking / capacity of judgement Time management and prioritization of tasks
Written communication competencies Selection and structuring Addressee orientation Visualization of content	**Teaching and educational competencies** Planning and designing courses Learning guidance / academic advising Supervision
Leadership competencies Strategic thinking and action Controlling team processes Conflict management	**Capacity for teamwork** Willingness to exchange information Capacity for collaboration and integration Consensus and solution orientation
Self-management Motivation, flexibility and commitment Dealing with criticism and opposition Self-marketing and networking	**Oral communication competencies** Presentation Argumentation / debating / asserting oneself
Creativity Generating ideas Implementing creativity outcomes	**Project management** Planning and monitoring Time and resource management Project communication

One step at a time

A PhD is proof of a relevant research achievement within a scientific community. In German-speaking countries you are awarded with a doctorate title ("Doktortitel"). The "Dr." in front of your name is often used in other (non-)professional surroundings and traditionally connoted with intelligence and integrity. When looking at higher management positions in German industry, "Doktortitel" appear frequently. This hints at a "glass ceiling", where career advancement might be gatekept for those, who achieved this title earlier in life. But right now, if you are seeking a foothold in the non-academic job market, further career steps are a long way down the road. In addition to the chemical industry, fields such as energy production, thermoelectrics, optoelectronics, conductors, analytical detection, medical technology, and surface coating may not yet realize they need your skills.

Will I be "overqualified"?

Entering a small or medium sized company (the workplace for more than half of university graduates) as "the doctor" might be even intimidating to your new peers. On one hand, the academic qualification level you acquired might not be required in daily business. Will you be bored? On the other hand, there are qualifications, certifications, and work experiences you obviously lack. Do you feel overqualified, underqualified or misqualified right now? Fortunately, you are a quick learner and the changing world of work is searching for talents. Outlining the tangible added value your PhD provides for your future employer right now might be a good idea. The German University Association of Advanced Graduate Training (UniWiND/GUAT) published a cluster with interdisciplinary competencies attributed to PhDs (see table 1) [2] which gives you a hint about the assets behind the title.

Dr. Julia Koppmann Ma. Sc. Chemistry
Career Service Universität Bielefeld
Universitätsstr. 25, D-33615 Bielefeld
julia.koppmann@uni-bielefeld.de
uni-bielefeld.de/career-service

Zurück zum Inhaltsverzeichnis

Did you recognize some of these competencies in your tasks? Great, they are proof of your professional skills. Do you feel this is not turning out as fruitful as it should at this point? Try to figure out how to incorporate more of the tasks you enjoy or would like to explore into your schedule. Identify the tasks you are looking forward to letting go of. If you are able to clarify your preferences, you will ultimately direct your job search in a more satisfying direction as an additional benefit. And when you feel comfortable with your future tasks, it shows in your application as well. That is probably what you call a win-win situation. Setting your PhD aside - browse your life for competencies you gained during voluntary work, vocational training, extracurricular trainings, or even a past study drop-out. Your CV is unique. Familiarize with current labor market vocabulary and find a way to translate your experiences to prove your fit.

Getting a good start

Do you have to do this all alone? Probably not! Get help from your university's career service, graduate center, your PhD supervisor or grad school administrator. Check your university's personnel development programs. Team up with others to share and save your information. Try to connect with graduates and find out about their jobs. Build a network. You are a scientist, and this is your personal research topic.

References

[1] Zentrum für Hochschulentwicklung, Datencheck 1/2023, hochschuldaten.che.de/promotionen-am-haeufigsten-in-naturwissenschaften-und-medizin/.

[2] Uniwind Publikationen Band 10, Kompetenzentwicklung von Nachwuchswissenschaftlerinnen und Nachwuchswissenschaftlern Fördern und Entwickeln, 2019.

Dr. Julia Koppmann Ma. Sc.

Julia Koppmann received her master's degree in chemistry in 2012 and her PhD in 2016 in the group of Katharina Kohse-Höinghaus from Bielefeld University. After completing her PhD she worked as a STEM program coordinator at the Bielefeld University Career Service. Since 2019, she has been working as a career advisor for doctoral students and postdocs.

ZITATBOX

„Der Doktortitel ist als Marathon anzusehen – lang, anstrengend, aber mit einem glorreichen Finale."

„Auf dem Weg zum Doktortitel werden Bücher zu deinen besten Freunden und Kaffee zu deinem treuesten Begleiter."

„Der lange Weg zum Doktortitel gleicht einer Reise ins Unbekannte – voller Herausforderungen, aber auch spannender Entdeckungen."

„Es braucht Ausdauer, Geduld und ein starkes Durchhaltevermögen, um bis zum Ende des langen Weges zum Doktortitel zu gelangen."

„Die Suche nach Antworten kann manchmal wie ein Labyrinth sein, aber der Doktortitel ist der ultimative Beweis dafür, dass du den richtigen Weg gefunden hast."

„Die Titelverleihung ist der Augenblick, in dem all die Nächte des Lernens und Forschens endlich belohnt werden."

„Mit dem Doktortitel in der Hand öffnen sich die Türen zu neuen Möglichkeiten und Abenteuern – lassen Sie die Reise beginnen!"

„Die Titelverleihung ist der stolzeste Moment, in dem Sie den Hut des Wissens aufsetzen und die Welt mit Ihrem Fachwissen beeindrucken."

„Der Doktortitel ist nicht nur ein Zeichen der Expertise, sondern auch eine Trophäe für den unermüdlichen Durst nach Wissen."

„Bildung ist der mächtigste Waffe, die wir verwenden können, um die Welt zu verändern." – Nelson Mandela

„Die wahre Entdeckungsreise besteht nicht darin, nach neuen Landschaften zu suchen, sondern mit neuen Augen zu sehen." – Marcel Proust

„Der Doktortitel ist nicht das Ende des Lernens, sondern erst der Anfang einer lebenslangen Wissensreise." – Unbekannt

„Das Streben nach Wissen ist ein nie endender Tanz zwischen Neugier und Entdeckung." – Albert Einstein

Quelle: https://coole-spruche.de/sprueche-doktortitel/

BUNSEN-MAGAZIN · 27. JAHRGANG · 1/2025

Johannes Dobbelaar

Career Opportunities for Chemists in Industry

When you want to study, what will it be? Is it worth studying chemistry?

The chemical industry is part of the manufacturing industry. It adds value to substances by converting them into new substances or materials. It is one of the largest global industries, ranging from oil and gas exploration all the way down to tailor-made medicine. Take chemistry out of our lives, and we will be thrown back many centuries in time. With more than 200 billion euros in revenue, the chemical industry is the third largest industry in Germany [1, 2, 3]. According to the German *Verband der Chemischen Industrie e.V.* [3], a bit less than half a million people work in the chemical and pharmaceutical industry, and this has been constant over the last 20 years. The chemical industry offers good wages [3] and is an attractive industry to work in.

Many students choose chemistry based on their passion for it, most likely not considering what they will do when they finish. Yet the question arises automatically when they get their degree. So what to do next? Now, depending on where you live, this is answered differently. In some countries, like the USA, it is quite common to start working after obtaining your bachelor's degree. In Germany, this is not that usual. Statistics [4] show that, once finished, 97% of chemistry bachelor's students automatically sign up for their master's. Approximately 85% [4] thereof even start their PhD. Almost 60% of those who finish their PhD start working in industry. Most of the remaining PhDs continue as postdocs or similar. So what is better for your career? PhD, master's or still bachelor?

I give you my personal observation of what determines the career development of a chemist in industry, be it bachelor, master, or PhD. Before that, it is important to note how long students take to achieve their degree. Studies from the GDCh [4] show that, on average, students need 3.5 years to obtain a bachelor's and between 2.5 and 3 years to obtain a master's degree. Those who continue their PhD need just a bit over 4 years to achieve this. A student needs around 10.5 years to finish with a PhD degree in chemistry.

In Germany, as mentioned, only a few students start working after their bachelor's. As a bachelor, you can start in jobs like production worker, routine testing and quality control, application testing etc. You compete with candidates with other degrees like lab technicians, associate chemists, or other chemistry degrees like the German "Chemikant." This will also determine your starting salary. With your master's degree in chemistry, you have learned to apply your chemistry knowledge. Your master's thesis is proof that you can complete assignments in a bigger project. You have learned to do experiments and analytics, or use simulation programs under guidance or even independently. You can summarize the work and conclude from it. Companies that require a master's degree look for people who can set up small projects based on customer demands, help optimize production processes, or develop testing methods for new samples. They expect you to work independently and be able to solve problems. Your knowledge will be rewarded with a higher starting salary than a bachelor's.

A PhD is the highest degree in chemistry education. With your thesis, you have proven to independently set up a research project and you are creative in solving complex problems. Companies often hire PhD students for their Research & Development. They will try to find those with a background in their chemistry. However, they know a PhD is capable of swiftly learning new chemistry and also hire PhD graduates who studied in another field of chemistry. They want you to advance their business by developing new products, new processes, etc. PhD students take on more responsibility and often start in a job where they lead a lab team or head a project team. Your skills are rewarded with a higher starting salary than masters.

Comparing the degrees, a PhD has the best starting position. However, we are not comparing the degrees equally. When starting a job, the bachelor's candidate will, on average, be about 6–6.5 years younger than the PhD candidate. How do they compare over time and age? Let us have a look at the following example where we compare three students of the same age taking different decisions during their study. Once the three achieve their bachelor's degree, one of them starts working as production worker, whereas the two peers continue their master's degree. After a few years, the one working may get the opportunity to change jobs and use his/her skills to become, e.g., process engineer. At the same time, the fellow students finish their master's degree and one of them starts working as a process manager. After several years, those working may have the opportunity to move to another position. Then the last of the three completes his/her PhD and starts working as lab leader in research.

So why go for a PhD when others can advance while they earn a salary?

The PhD is a qualification that gives access to a higher entry level in a company with appropriate higher salary and often

Dr. Johannes Dobbelaar
BASF SE
Carl-Boschstraße 38, D-67056 Ludwigshafen am Rhein
johannes.dobbelaar@basf.com

Zurück zum Inhaltsverzeichnis

higher responsibility. Though the other two can advance to this level as well, my observation is that it takes them longer to get there. They can advance their career in industry when they invest in acquiring experience, upgrade their knowledge by following additional training and courses, and change to appropriate jobs. As a PhD, however, you have qualifications which make the spectrum of entry jobs larger, because some jobs will be advertised to PhD holders only. And, starting from a higher level, you can also advance in your career by acquiring additional skills.

Now that leaves the question: "Does it financially pay out to do your PhD?"

During your PhD your income will be lower than those bachelors and masters who work in the industry at the same time. As a PhD working in industry, your starting salary will typically be higher than the salaries both others have advanced to by then. Will you be able to financially stay ahead of the bachelor and master during your working life? The answer to this question will come shortly since there is more to know.

What happens with the three fellows during the rest of their career?

This only partly depends on their education level. Though the PhD has the advantage of the higher degree and the capabilities, there are more skills needed to advance in the industry. You can specialize and even become a real expert in your field. When your knowledge and skills are wanted, you will be rewarded for that. You follow a specialist career. Another way is a generalist career, where you advance into management and maybe into leadership. Here not only decent technical knowledge is needed, but also a good network, strategic thinking, leadership skills, communication skills, business management, drive, persuasion, etc. These skills are not taught at university, but you can acquire them in and next to your job. All three fellows are able to pursue either one of the career paths. It depends on their personal ambition, how much time and effort they put into acquiring the necessary skills. With smart moves and diligence you can even advance all the way to CEO level. Check out the background of several company leaders you know and see what education levels they have and how they advanced their career.

Thus with career advancement, you will also financially significantly advance beyond entry level positions. If you don't know whether or what career path you want to pursue, you can talk to a coach. If you don't know how to develop your career, you can talk to a mentor as well. Though, achieving your career aspirations depends on your own action.

To conclude, the way I observe it is that your degree will determine which starting positions are open to you and what your starting salary is. Your personal ambition and action will determine how much you advance your career and how much you are rewarded for it. To drive your own career and differentiate yourself financially, you should have an idea of what you are aiming for and how much time and effort you want to invest to achieve it.

References

[1] Technik und Wirtschaft für die deutsche Industrie. Produktion 29. April 2024, Stefan Weinzierl. Industrie: Das sind die wichtigsten Branchen in Deutschland. www.produktion.de.

[2] Industrieland Deutschland – die wichtigsten Fakten 24. Juli 2023, Martin Orth. www.deutschland.de.

[3] VNCI, Chemiewirtschaft in Zahlen online. Chemiewirtschaft in Zahlen online | VCI.

[4] The GDCh statistics on chemistry courses (flip catalog) 2023. Blätterkatalog (gdch.de).

Dr. Johannes Dobbelaar

Dr. Johannes Dobbelaar, Vice President Global Technology Dispersions, Resins and Additives at BASF SE, brings over 30 years of business experience in various operational roles. He has successfully managed teams across multiple countries and continents, showcasing his expertise in organisational development and strategic growth. Now, as the leader of global process technology, he drives capital investments for growth and enhances the asset footprint with respect to sustainability and digitalization.

Perspectives on PhDs in Industry

As opposed to PhDs in academia, industry PhDs are far less common and most prospective PhD students do not know much about them. How does a PhD in academia differ from one in industry? What are the advantages and what are the challenges of industry PhDs? We as yPC wanted to know more so we asked Dr. Uwe Nickel, former chair of the DBG, about his perspective as an industry expert as well as Dr.-Ing. Lisa Büker, who has carried out an industry PhD.

yPC Editorial Team

Uwe Nickel

Die Industriepromotion – Eine Alternative ?

Seit Jahrzehnten gibt es das ungeschriebene Gesetz, dass ein Start in der chemischen Industrie am aussichtsreichsten mit einer abgeschlossenen Promotion einhergeht. Dies ist zumindest in den meisten westlichen Staaten und den großen Industrieunternehmen die Regel. Mit der Erfahrung und dem Rückblick auf eine lange und diversifizierte Industriekarriere frage ich mich seit vielen Jahrzehnten, warum das immer noch so ist und warum sich das nicht wesentlich verändert hat. Denn viele promovierte Chemiker sind erstaunt, dass sie in dem Industrieunternehmen dann zwar in Forschung und Entwicklung (F&E) als einer der Ausgangspunkte einer Industriekarriere starten, aber nur begrenzt mit den Themen zu tun haben, für die sie viele Jahre im Studium gearbeitet haben. Das ist dann der zweite Praxisschock im Leben, nach dem Übergang von der Schule an die Universität. Volks- und betriebswirtschaftlich ist es durchaus diskutierwürdig mal nach dem Sinn einer Promotion vor dem Start in die Industrie zu fragen, wenn man dann meist etwas ganz Anderes in der Industrie macht. Dass dies mehr als eine theoretische Überlegung ist, zeigen die reinen Fakten. Nach der Statistik der GDCH dauert die Zeit bis zur Promotion, die immerhin 434 Studenten in 2023 machten, über 20 Semester. 57% davon haben dann eine Anstellung in der Wirtschaft bzw. 40% in der chemischen Industrie gefunden. Also lohnt es sich, Alternativwege zu betrachten. Ein Masterstudium dauerte 2023 in der Regel 12 Semester und 67% der Absolventen gingen in die Industrie. Wir reden also von vier bis fünf Jahren, die man gegebenenfalls optimierter und Themen fokussierter einsetzen kann, von den Verdienstmöglichkeiten mal ganz zu schweigen. Eine Promotion vor Beginn einer Industriekarriere hat viele Vorteile. Man lernt das selbständige wissenschaftliche Arbeiten, Durchhaltevermögen/Ausdauer und strukturiertes teilweise projektbezogene Arbeiten und Handeln. Das sind alles Werte neben den inhaltlichen Dingen, die essenziell sind für eine erfolgreiche Industriekarriere. Allerdings haben die wenigsten eine Vorstellung von dem, was sie in der Industrie dann erwartet. Die Industrie ihrerseits ist zwar an exzellenten Absolventen interessiert, aber wirtschaftlicher Erfolg auf Basis ausgezeichneter wettbewerbsfähiger Produkte steht im Vordergrund und nicht jeder Absolvent mit einer exzellenten Promotion entpuppt sich dann auch als exzellenter und förderungswürdiger Mitarbeiter.

Hier kommt dann die Industriepromotion ins Spiel. Viele Unternehmen hadern nach wie vor mit dieser Option aber auch viele Studenten. Dieser duale Weg ist aber längst nichts Exotisches mehr. Es ist durchaus gang und gäbe, dass Mitarbeiter von Industrieunternehmen einen MBA während Ihres Berufs machen. Das bindet die Mitarbeiter an Unternehmen und das Unternehmen investiert in Menschen, die sie schon kennen. Ein MBA ist keine Promotion, aber der Ansatz ist ähnlich. Der große Unterschied ist, dass man für eine Industriepromotion zunächst einmal eine enge Kooperation zwischen einer promotionsberechtigten Hochschule und dem Industrieunternehmen haben muss. Dann bedarf es eines hohen Abstimmungsaufwandes zwischen der Professur und dem Industriebereich. Was dann nicht zu unterschätzen ist, ist die Doppelbelastung, sprich Job einerseits und Promotion andererseits. Das ist nichts für ein bis zwei Jahre, das dauert und bedarf eines langen Atems sowohl vom Promovierenden, aber auch vom Unternehmen, denn die Anforderungen an eine Promotion müssen mit den betrieblichen Zwängen und der Karriereentwicklung in Einklang gebracht werden. Gängige Karriereschritte und der oftmalige Sprung zwischen Bereichen, also von F&E in Produktion oder Marketing oder die kurzfristige Entsendung ins Ausland, sind dann schwer zu planen und praktisch kaum umzusetzen.

Doch es hat Vorzüge. Man ist wirtschaftlich abgesichert, wenn man den Weg der Industriepromotion geht. Man ist bereits Teil eines Unternehmens und Teil der Kultur und nicht der 29–32-jährige Neuling, der zwar promoviert ist, aber noch nie ein Unternehmen (es sei denn, sie/er macht Exkurse und engagiert sich in yPC) von innen gesehen hat. Man kann sowohl von Arbeitgeber- als auch von Arbeitnehmerseite entscheiden, ob eine Promotion passt oder nicht – das reduziert potenzielle Enttäuschungen auf beiden Seiten. Heutige Karrieren in Chemieunternehmen sind

Dr. Uwe Nickel
Proventis Partner AG
Zürich
Switzerland
u.nickel@proventis.com

schon lange nicht mehr vom „Dr.“-Titel abhängig. Es zählen breite Kenntnisse, Flexibilität, die Mischung aus naturwissenschaftlichen, Management und betriebswirtschaftlichen Kenntnissen. Eine Industriepromotion hat auch den Vorteil, dass man an einem Thema arbeitet, welches eine hohe praktische Relevanz hat und eine hohe Chance auf direkte Umsetzung. Volkswirtschaftlich und betriebswirtschaftlich ist das ein Plus, denn es ist ein Unterschied, ob man mit 24 oder mit 29-32 in die Industrie einsteigt. Das sind bei einer durchschnittlichen Industriearbeitszeit von 35 Jahren dann 15% an Gewinn.

Fazit: Nicht nur innovative Erfindungen und Entwicklungen wagen und machen, sondern auch mehr innovative bedarfsorientierte Personalentwicklungswege gehen.

Dr. Uwe Nickel

Dr. Uwe Nickel startete seine Industriekarriere nach Studium und Promotion der Chemie in Frankfurt am Main bei der Cassella AG in 1986. Nach kurzem Aufenthalt in der Forschung, wechselte er in die Tenside- und Pharmaproduktion. Nach einer Stabsstellenzeit als Vorstandsassistent wurde er Abteilungsleiter in die Produktion, bevor er 1995 zur Hoechst AG wechselte. 1996 wechselte er infolge des Verkaufs des Bereichs Spezialchemikalien von Hoechst zum Schweizer Konzern Clariant in Basel. Dort durchlief er verschiedene internationale Stationen im Bereich Pigmente & Additive, bevor er 2003 in den Vorstand des Unternehmens berufen wurde. Von 2007 an arbeitete er bei der Unternehmensberatung Arthur D. Little und wurde 2010 CEO der HCS Group, einem mittelständischen Spezialchemieunternehmen. Von 2017-2018 war er Erster Vorsitzender der DBG. Ab 2020 baute er als Partner den Chemiesektor der Proventis Partners AG, einem auf M&A spezialisiertem Unternehmen in Zürich auf. Neben dieser Tätigkeit begleitet er noch einige Beiratsmandate in Mittelstandsunternehmen und agiert als Investor in der Agro- und Chemiesparte. Uwe Nickel lebt bei Basel, ist verheiratet und hat vier Kinder.

That's yPC!

“I am eager to collaborate with young physical chemists and contribute creatively to exciting projects!”

Ekaterina Salikhova is a PhD candidate at the Fraunhofer IAP-CAN & University of Hamburg. She works on novel synthesis strategies for RoHS-compliant, IR-active nanoparticles.

Join yPC and shape the future of the Physical Chemistry Community!

Do you like to **work in a team**?
Are you **creative** or like to **connect to others**?
Then join the **young Physical Chemists**!

Our goals:
Connect early career scientists!
Represent their interests in and outside DBG!
Support them in their career development!

Interested? Get in contact!
ypc@go.bunsen.de

young PHYSICAL CHEMISTS

Lisa Büker

Doing Your PhD in Industry – An Experience Report

Already during my school time, I realised that I wanted to work in the natural sciences. That's why I trained as a chemical laboratory technician at a company specialising in electroplating technology after leaving school. As the knowledge I had acquired during my apprenticeship was not enough for me, I studied chemistry. At the end of my master's degree, a former colleague told me that the company KIESOW OBERFLÄCHENCHEMIE (North Rhine-Westphalia, Germany) was looking for someone to do a doctorate in collaboration with the Technical University of Ilmenau (Thuringia, Germany). As KIESOW OBERFLÄCHENCHEMIE is a company that specialises in the field of electroplating, just like my training company, I was interested right from the start.

During my PhD, I was employed by KIESOW OBERFLÄCHENCHEMIE and registered as a PhD student at the Technical University of Ilmenau in the 'Department of Electrochemistry and Electroplating'. My contract stipulated a 40-hour week, so I worked 20 hours for KIESOW OBERFLÄCHENCHEMIE and had 20 hours per week for my thesis. It was clarified between KIESOW OBERFLÄCHENCHEMIE and the TU Ilmenau that the data obtained in the context of publications would not be subject to a certain degree of confidentiality. This is an important decision to be discussed at the beginning of an industrial PhD, before complications arise afterwards.

Both the company and the university gave me a lot of support throughout my doctorate. It was clear from the start that successfully completing my PhD thesis was the main concern, so I was able to use my time for the doctorate beyond the 20 hours. At the TU Ilmenau there is a doctoral seminar in which the university doctoral students and the industry doctoral students have the opportunity to get to know each other. This enabled us to establish contact and a good dialogue. The collaboration with the working group is still very close and friendly today. Many of my fellow students who started their doctorate in industry did not finish it because they were not given enough time or were distracted by the company's work. The PhD thesis must always have the highest priority. One of the most important things I learned during my doctorate was how to work independently and find solutions to problems; my frustration thresholds were expanded. You also learn how to work in industry, where tight schedules and pressure determine everyday life. Besides, I was able to meet many different people and experience different ways of interacting. I got to know many different personalities, from production employees to senior managers. I had to learn to adapt to all of them. At university, you work with people who have similar aspirations and goals. It was a change for me to work with people who were less motivated and less structured, but it was a challenge to find ways and means to make the projects work. As a woman in a male-dominated industry, you need a thick skin. For me personally, it was always a good way not to be too "*sensitive*". But you still have to learn to assert yourself and not put up with everything. In contrast to pure basic research, which is often carried out at universities, during my industrial doctorate I was able to work on a topic that is of interest to the company and numerous users. I therefore gained a lot of experience through contacts with customers and suppliers of raw materials. My direct supervisor at the company was always a great help and an important contact person. He gave me the space I needed and did everything in his power to give me the support I needed. Moreover, the exchange with my fellow students was also excellent, my professor and the students were always very supportive. Despite the distance, I was always supported with my measurements, doctoral planning and publications. As I was very lucky with the company and the university, I wouldn't want to change my decision to do a doctorate in industry. The advantage of an industrial doctorate is that you get a direct insight into the industry and can make contacts. I was able to experience the different fields, perspectives and working methods, which will hopefully give me the opportunity to deal with challenges in my future career. After finishing my PhD studies, I was taken on by KIESOW OBERFLÄCHENCHEMIE and was able to take on a management position in the company straight away.

Dr.-Ing. Lisa Büker
Kiesow Oberflächenchemie GmbH & Co. KG
Wittekindstraße 27 – 35, D-32758 Detmold
l.bueker@kiesow.org

Dr.-Ing. Lisa Büker

Lisa Büker is Product Manager at Kiesow Oberflächenchemie GmbH & Co. KG in Detmold and is responsible for the Decorative Department. As part of this responsibility, she is in charge of communication between the back office and the sales force. The coordination of the development team in cooperation with the laboratory management is an important aspect of this. In the area of decorative development, the focus is on copper, nickel and chrome electrolytes. She began her professional career with an apprenticeship as a chemical laboratory assistant before starting a chemistry degree at the University of Bielefeld in 2011. She successfully completed this with a Master of Science in January 2017. Immediately afterwards, she began her doctorate in Electrochemistry & Electroplating at the TU Ilmenau in collaboration with Kiesow Oberflächenchemie. She successfully completed her doctorate in 2022.

Christian Zocher, Berthold Kersting

Doing a PhD as Part of an SFB (Collaborative Research Center, CRC)

Pursuing a PhD within a Collaborative Research Center (CRC, or *Sonderforschungsbereich* (SFB) in Germany) offers a unique, interdisciplinary environment that can make the demanding process of completing a doctorate both more manageable and professionally enriching. CRCs, funded by the German Research Foundation (DFG, or *Deutsche Forschungsgemeinschaft*), are long-term research programs uniting researchers across institutions and fields around a common research theme. For PhD students, this structure brings numerous advantages, offering both resources and a vibrant collaborative network that can greatly enhance the doctoral experience.

One of the main benefits of doing a PhD in a CRC is the access to interdisciplinary research. With a CRC, you're not limited to your immediate field; rather, you work alongside experts from other areas, often across institutions. For instance, a PhD student in chemistry might collaborate with specialists in physics, biology, experimentalists or theorists, learning new methods and approaches that might otherwise be difficult to access in a traditional, single-discipline PhD program. This interdisciplinary approach broadens the scope of research possibilities and equips doctoral candidates with a wider scientific perspective. The financial support available in CRCs is another major advantage. Unlike independent PhD programs, CRCs typically provide ample funding for conferences, workshops, and advanced training sessions. These opportunities are not only beneficial for expanding one's knowledge base but are also essential for networking with international researchers. Conferences and training sessions allow PhD students to present their work, discuss ideas, and connect with leading scientists from around the world. This fosters international collaborations and offers insights into global research trends. However, taking full advantage of these opportunities requires initiative from PhD students to seek out the most relevant events to attend and planning their attendance.

Another valuable aspect of a CRC is the strong peer network it fosters. Typically, multiple PhD students begin their projects in the same cohort, providing an immediate community of peers. This shared experience can be especially helpful, as it allows students to exchange ideas, seek feedback, and navigate common challenges together. Many CRCs also include integrated graduate programs, which encourage interdisciplinary training and help establish a shared scientific language across fields. This not only aids in effective communication but also strengthens collaboration within the group.

Despite the many advantages, participating in a CRC also comes with unique challenges. Networking is crucial to the CRC experience, but it demands considerable time and effort. Coordinating with numerous partners – some of whom may be based in different countries – requires patience, time management and strong communication skills. Additionally, the collaborative structure of CRC projects often requires a higher level of commitment than a traditional PhD. Regular status updates, project discussions, and colloquia are standard, meaning that PhD students must frequently present their findings and discuss their progress with supervisors and other researchers. Although these presentations provide valuable feedback, they also add to the workload and require continuous refinement of communication skills.

Furthermore, the interdependent nature of CRC projects necessitates careful planning and coordination. In many cases, progress in one project is contingent on the results from another, creating a chain of dependencies that requires synchronized timelines. While this structure can be challenging, it instills project management skills and cultivates a strong sense of responsibility and teamwork. Ultimately, doing a PhD within a CRC entails additional responsibilities, but the rewards – including access to resources, networking opportunities, and interdisciplinary training – make it a valuable and enriching experience. For those willing to embrace both the challenges and the unique advantages, a CRC offers a solid foundation for a career in research and beyond.

M. Sc. Christian Zocher
Prof. Dr. Berthold Kersting
Institut of Inorganic Chemistry and Crystallography
Universität Leipzig
Johannisallee 29, D-04103 Leipzig
christian.zocher@uni-leipzig.de
b.kersting@uni-leipzig.de
https://www.chemie.uni-leipzig.de/institut-fuer-anorganische-chemie-und-kristallographie/arbeitskreis-kersting

HYP*MOL
HYPERPOLARIZATION IN MOLECULAR SYSTEMS
POLARIZATION | TRANSPORT | REACTIVITY

Logo of the CRC HYP*MOL (Copyright: HYP*MOL). „Funded by German Research Foundation (DFG), TRR-386, project number 514664767."

M. Sc. Christian Zocher

Christian Zocher received his Bachelor's degree in chemistry in 2019 in Leipzig. During his master studies, he participated in an exchange program at Jyväskylä University (JYU) Finland. He received his master's degree in chemistry in 2023 and his master's degree in mineralogy, crystallography and material science in the same year in the group of professor Kersting from Leipzig University. He then accepted a PhD position in 2023 in the same group.

"Welcoming the young Physical Chemists of the German Bunsen Society for Physical Chemistry to EYCN/EuChemS" - check out our article in the EuChemS Magazine Plus here! https://www.magazine.euchems.eu/bunsen-eycn/

Wilhelm Jost Memorial Lecture 2024

In memory of Wilhelm Jost and to promote physical chemistry, particularly in the interdisciplinary field of ecology, the Göttingen Academy of Sciences and Humanities awards the Wilhelm Jost Memorial Lecture to outstanding physical chemists. In accordance with the statutes, the prizewinner gives lectures at selected places where Wilhelm Jost lived: the universities of Halle, Berlin, Hanover, Leipzig, Marburg, Darmstadt and Göttingen. The Bunsen Society proposes suitable candidates to the Göttingen Academy.

Dr. Nils Hansen of the Combustion Research Facility, Sandia National Laboratories, Livermore, California, USA was awarded the Wilhelm Jost Memorial Lecture 2024 by the Göttingen Academy of Sciences and Humanities. Dr. Hansen lectured on *Chemical Kinetics in Multiphase Chemical Transformation* in Darmstadt, Hannover, Halle, Leipzig and Marburg. He was awarded the Wilhelm Jost Memorial Medal on 29th October 2024 in Göttingen.

Lecture abstract

Wilhelm Jost is particularly renowned for his contributions to the field of chemical kinetics and reaction dynamics. He has made significant advancements in understanding of how chemical reactions occur during combustion, which is critical for various applications ranging from industrial processes to energy production and environmental science. His work continues to support today's development of and transition to clean and energy-efficient chemical transformations.

Continuing and expanding of the foundational principles established by Wilhelm Jost, our team has applied mass spectrometric approaches to provide basic insights into chemical kinetics of reaction networks of complex environments and applications. The first part of the talk focuses on new chemical insights into molecular-weight growth and soot formation chemistry in combustion processes by reactions of resonantly stabilized radicals. The second part of the talk focuses on reaction networks found in catalytic heterogeneous chemical transformations. Specifically, we will highlight new insights into gas-surface interactions during catalytic partial oxidation of methanol and oxidative coupling of methane with soft oxidants. The last part highlights how non-equilibrium plasma can initiate chemical conversion through the generation of charged species, radicals, and excited-state species. We will discuss examples from plasma-assisted chemical looping combustion and methane dry reforming.

Photo from left to right: Prof. Dr. Oliver Bünemann, GDCh-Ortsverband Göttingen, Dr. Nils Hansen, Award Recipient, Prof. Dr. Kurt Schönhammer, Göttingen Academy of Sciences and Humanities, Prof. Dr. Alec Wodtke, Representative of Physical Chemistry in Göttingen. Copyright: Arved Dorst.

Javier García-Martínez

How To Make the Most of your PhD?

The Spanish physician and scientist Santiago Ramón y Cajal (1852-1934), considered the father of modern neuroscience and winner of the 1906 Nobel Prize in Physiology or Medicine, is the author of a short but highly recommended book entitled "Reglas y Consejos sobre Investigación Cientifica: Los tónicos de la voluntad", which in English is usually loosely translated as "Advice for a Young Investigator" (Figure 1) [1]. In it, he offers a series of valuable pieces of advice to young researchers, based on his own experience as a scientist. This short and very entertaining book is particularly useful if you are considering starting a PhD, or if you are at the difficult moment of trying to make sense of all the work you have done after years of research in the lab, writing your thesis.

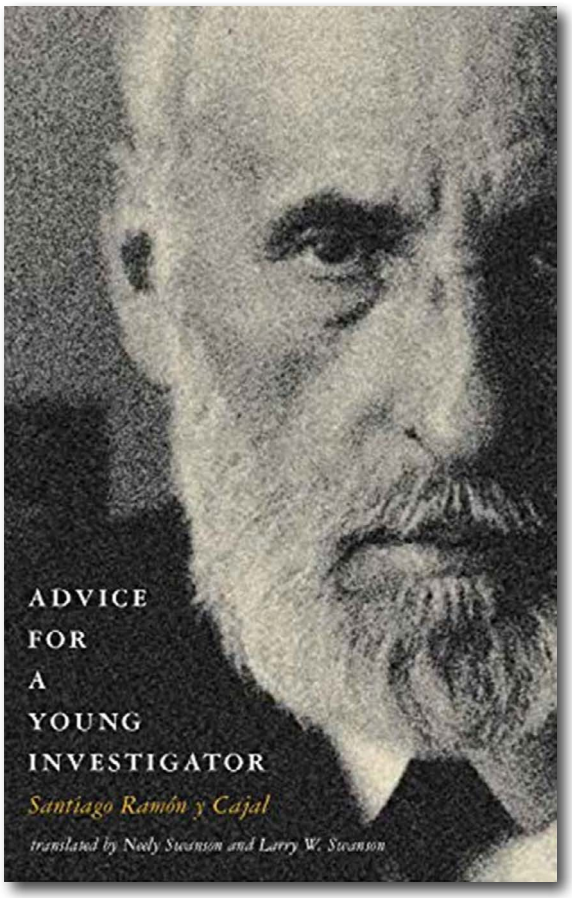


Fig. 1: Cover of the book: Advice for a Young Investigator. (Santiago Ramón y Cajal)

Prof. Dr. Javier García-Martínez
Department of Inorganic Chemistry
University of Alicante
Carretera San Vicente s/n, 03690, Alicante, Spain
j.garcia@ua.es

Some of the ideas I share in this short article, which Noah Al-Shamery – current Communications Team Leader and Board Member of the European Young Chemist Network (EYCN) and Co-Speaker of the young Physical Chemists (yPC) of the German Bunsen Society for Physical Chemistry – asked me to write, can be found in this little book packed with useful lessons and many personal anecdotes. These are just some of the practical tips that Santiago Ramón y Cajal shares with the "young investigator":

1. Cultivate patience and perseverance
Be patient and perseverant in your scientific work. Science is a field full of difficulties and failures; therefore, it is necessary to be prepared to endure moments of discouragement and frustration, always maintaining perseverance in research.

2. Develop solid self-discipline
Foster your self-discipline, which includes the ability to concentrate on a single line of research, avoiding dispersion and temporary enthusiasm for several topics at once. Organise your time rigorously and establish a methodical working routine to achieve success in research.

3. Encourage curiosity and critical thinking
Curiosity is one of the fundamental virtues of the scientist. It is key to keep an open mind, to constantly question existing data and theories, and to develop a critical spirit that allows one to go beyond what is known, always searching for the truth with rigour.

4. Maintain a humble and dispassionate attitude
Young researchers should maintain intellectual humility and recognise their own limitations and mistakes. It is crucial not to be carried away by vanity or fame, but to pursue knowledge for the mere fact of contributing to the advancement of science.

5. Strive for originality and independence
Be original and develop your own thinking, avoiding imitation or excessive dependence on the ideas of others. Cultivate your intellectual independence, question established doctrines and develop your own theories.

6. Value collaboration and communication
Independence is important, but so are teamwork and scientific collaboration. Share your findings with the scientific community, be open to the exchange of ideas, to criticism and to learning from others.

7. Take care of your physical and mental health

You should maintain a balance between work and health, taking care of both your physical and mental wellbeing. Scientific research requires a great deal of energy and stamina, and it is essential to maintain a healthy body and mind. After reading this book, you will conclude that a doctorate is not for everyone, but if you decide to embark on this intellectual adventure, you will learn to think critically, to propose hypotheses and to discard those that do not stand up to experimental evidence. You will develop dedication, discipline and a passion for truth. Santiago Ramon y Cajal's advice is timeless and applies not only to scientific research, but also to anyone who is committed to the quest for knowledge.

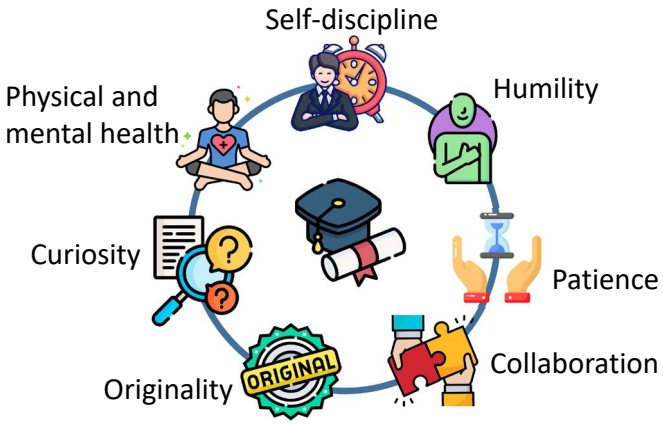


Fig. 2: Traits of a successful PhD student, inspired by Santiago Ramón y Cajal. (CC0)

A short guide for a successful PhD

Choosing and successfully completing a PhD programme involves several steps, starting with a personal reflection on your passions, academic interests and long-term career goals. Only through this process of self-reflection will you be able to choose a research topic that not only excites you, but also has substantial academic significance and potential for real-world impact. This topic should ideally be in line with emerging trends in your field and offer opportunities for original contributions to knowledge. It's also important to consider the feasibility of your research, taking into account the resources available, your own background and the scope of the PhD project [2].

The next step is to find a suitable supervisor, which can be one of the most important decisions of your doctoral journey [3]. Look for someone who is not only an expert in your chosen field, but also someone whose mentoring style matches your needs and personality. A supportive and approachable supervisor can provide critical guidance, open doors for you and help you overcome the challenges you'll face. Look for professors who are actively publishing, have a solid track record and a strong academic network, but who are also enthusiastic about mentoring doctoral students. Talk to other PhD students and former members of the lab, but remember it takes two to tango, so put your best foot forward to create a healthy and enriching experience with your supervisor.

Once enrolled, the success of your PhD depends to a large extent on effective time management and a well-structured research plan. Most doctoral students tend to procrastinate, believing that there is always time. I strongly recommend that you set clear, achievable milestones and break your work down into manageable tasks, with clearly defined milestones and times, to avoid feeling overwhelmed, but also to avoid procrastination. Regularly reviewing and adjusting your plan in consultation with your supervisor is key to staying on track. Make use of the resources offered by your institution, such as workshops on research skills, academic writing and career development. Attending seminars, conferences and academic events will help you keep abreast of developments in your field and build a professional network. Technology can also help. Used wisely, an increasing number of online tools and apps can help you better manage your time, meet deadlines and streamline some of the most time-consuming tasks [4].

A PhD journey is often fraught with challenges, including moments of self-doubt, setbacks in research, or even unexpected results. Cultivating resilience and maintaining a positive attitude are vital. Learn to see challenges as opportunities for growth rather than obstacles. Seek feedback constructively, and be prepared to revise your work multiple times; this is a normal part of the academic process. Balancing work with self-care is crucial to avoid burnout; ensure you have a support system in place, whether through friends, family, or fellow PhD students.

If your research leads to a scientific discovery, technology or service with potential for commercialisation, you should consider this option if it fits your personality and aspirations [5]. To do this, start by identifying a market need that matches your research, and then develop a business model that demonstrates how your innovation can meet that need. Building a strong network of mentors, advisors and potential collaborators – including faculty members and industry experts – is crucial to navigating the path from academia to industry. Protecting your intellectual property through patents or other legal rights can be a significant competitive advantage. Make sure you take advantage of what your institution has to offer in this area and find out more about IP protection and licensing. While entrepreneurship is not traditionally a focus of most doctoral programmes, it is gaining traction as a powerful way to create value, make a real impact and showcase the full potential of your research.

Finally, remember that a PhD is not just about producing a dissertation, it is about developing a comprehensive set of research, critical thinking and problem-solving skills. Engage with your research community, both online and in person by attending the main conferences in your field, build your academic profile by publishing high quality work, and consider the wider impact of your work. By remaining curious and open to new ideas, you will not only increase your chances of success in your doctoral programme, but also prepare yourself for a rewarding career in academia and beyond [6]. So, explore topics beyond your usual focus, keep up with the latest scientific news and learn to connect seemingly unrelated concepts, all of this will help you seeing the bigger picture, a quality that is essential to making a real impact in science.

References

[1] Santiago Ramón y Cajal, Neely Swanson, Larry W. Swanson: *Advice for a Young Investigator*, The MIT Press, 2004.

[2] Twenty things I wish I'd known when I started my PhD, *Nature*, accessed 27/08/2024. Available at: https://www.nature.com/articles/d41586-018-07332-x

[3] How to choose the right PhD supervisor, *Nature Index*, accessed 27/08/2024. Available at: https://www.nature.com/nature-index/news/how-to-choose-the-right-phd-supervisor

[4] Five online tools that aim to save researchers time and trouble, *Nature Index*, accessed 27/08/2024. Available at: https://www.nature.com/nature-index/news/five-online-tools-that-aim-to-save-researchers-time-and-trouble

[5] J. Garcia-Martinez, K. Li: *Chemistry Entrepreneurship*, Wiley-VCH, 2021.

[6] M. Jagodic, P. Stridh, A. Gad, et al.: Nurture your scientific curiosity early in your research career, *Nature Genetics* 2013, **45**, 116–118. https://doi.org/10.1038/ng.2527

Javier García-Martínez

Go Beyond the Lab

This is not the first time I have been asked to write an article for early career researchers and share my experiences, advice and thoughts. In 2021, I wrote the article "Standing on the Shoulders of Giants – Your Mentors and Role Models Will Shape Your Career" for the Science Voices section of Chemistry an European Journal [1]. In this article I shared some advice based on my experience as a volunteer for more than 15 years at the International Union of Pure and Applied Chemistry (IUPAC). The following are seven reasons I gave in the article for combining your research with volunteer work in an international organisation.

1. This experience gives you the opportunity to work in a very diverse environment where cultural differences, priorities and even world views are as diverse as it gets. There are few better ways of seeing the bigger picture than this.

2. As a volunteer in a large scientific organization, you will develop many soft skills including empathy and open-mindedness; but, at the same time, you will have to learn how to keep your priorities and advance your own program.

3. You will learn how to teamwork, delegate, and, above all, to rely on like-minded people to carry out the projects that are most important to you.

4. You will discover international programs and career opportunities that otherwise tend to go unnoticed.

5. You will come into contact with many people working in a number of global organizations who may become great professional contacts in the future.

6. You will have the opportunity to shape your field and make a difference in the world by working on those projects or initiatives that are more aligned with your passion.

7. Serving in an international scientific organization is a fantastic way to make friends from around the world who share your same interests.

I am sure that Noah Al-Shamery or any other EYCN volunteer could share their own reasons for choosing to take time out of their busy lab schedules to volunteer in international organisations. With this in mind, I would like to share some additional reading that they have found useful – written by members of the International Young Chemistry Network (IYCN) and its European sister network EYCN – [2-4] where you can learn more about their own personal and professional development and how they are making a real impact beyond their research.

Mentors and role models will make your journey smoother and more successful

I cannot help but comment on an idea I discussed in my article "Standing on the Shoulders of Giants", namely the importance of choosing and nurturing relationships with good mentors. This advice comes from my own experience. I have seen first-hand how important it is to benefit from the advice and support of those who have walked the path before you. So, I include here the tips I shared in that article to identify the most suitable mentor for you.

Prof. Dr. Javier García-Martínez
Department of Inorganic Chemistry
University of Alicante
Carretera San Vicente s/n, 03690, Alicante, Spain
j.garcia@ua.es

1. Read biographies to discover new and interesting people and how they made difficult decisions and the resources they used.

2. Learn more about the lives of great people who made significant contributions to your field. Most likely they had to face similar challenges to the ones we will have to overcome.

3. Realize that every person has their lights and shadows. A role model is not by any means a perfect individual. It is a person who exemplifies some of the values we want to live for and made some difficult decisions that can serve you as an inspiration when you have to face similar challenges.

4. Identify the values that are more important to you and find the people who have lived according to those principles.

5. Ask yourself what your role model would have done in a particular situation, and if that answer helps you to make a difficult decision and to become a better person and advance in your career, that role model is probably right for you.

Finally, I would like to return to my first piece of advice. Reading biographies is crucial for two reasons, it humanises science and it provides valuable perspective. When you learn that even the greatest figures in science have faced significant challenges and still made remarkable contributions to humanity, it becomes clear that you, too, can overcome any obstacles you may face - whether during your PhD or at any point in your career. Remember the words of the American educator Booker T. Washington: “Success is to be measured not so much by the position that one has reached in life as by the obstacles which he has overcome while trying to succeed [5].”

Prof. Javier García-Martínez

Professor of Inorganic Chemistry and Director of the Molecular Nanotechnology Laboratory at the University of Alicante, Spain.

President of the International Union of Pure and Applied Chemistry (IUPAC) for the 2022-23 biennium.

His contributions to nanotechnology have unlocked the potential of heterogeneous catalysts for the conversion of bulky molecules by introducing controlled intracrystalline mesopositivity. This technology is now widely used in academic laboratories and chemical companies around the world, saving hundreds of thousands of tonnes of CO_2 per year by reducing the amount of waste and coke that would otherwise be burned to produce green gas emissions in key industrial processes ranging from biomass conversion to catalytic cracking.

His contributions to catalysis, energy and chemistry have been recognised with some of the most prestigious awards including the Kathryn C. Hach Award for Entrepreneurial Success from the American Chemical Society, he is an Honorary Fellow of the Royal Society of Chemistry and earlier this year received the National Research Award from the King of Spain.

References

[1] J. García-Martínez: *Chem. Eur. J.* 2021, **27**, 13664.

[2] EYCN and IYCN: Connecting and Empowering Young Chemists Globally, *Chemistry Views*, accessed 27/08/2024. Available at: https://www.chemistryviews.org/details/ezine/11226971/EYCN_and_IYCN_Connecting_and_Empowering_Young_Chemists_Globally/

[3] T. John, K. E. Cordova, C. T. Jackson, A. C. Hernández-Mondragón, B. L. Davids, L. Raheja, J. V. Milić, J. Borges: *Angew. Chem. Int. Ed.* 2023, **62**, e202217841.

[4] E. Dobbelaar, S. S. Goher, J. L. Vidal, N. K. Obhi, B. M. B. Felisilda, Y. S. L. Choo, H. Ismail, H. L. Lee, V. Nascimento, R. Al Bakain, M. Ranasinghe, B. L. Davids, A. Naim, N.-A. Offiong, J. Borges, T. John: *Angew. Chem. Int. Ed.* 2024, **63**, e202319892.

[5] Booker T. Washington: *Up from Slavery: An Autobiography*, 1901.

ZITATBOX

Thomas Alva Edison

„Der sicherste Weg zum Erfolg ist immer, es doch noch einmal zu versuchen.“

Willy Brandt

„Kleine Schritte sind besser als keine Schritte.“

Immanuel Kant

„Der Ziellose erleidet sein Schicksal – der Zielbewusste gestaltet es."

Johann Wolfgang von Goethe

„Erfolgreich zu sein, setzt zwei Dinge voraus: Klare Ziele und den brennenden Wunsch, sie zu erreichen."

Martin Luther

„Wer einen Misserfolg nur als kleinen Umweg betrachtet, verliert nie sein Ziel aus den Augen."

Quelle: https://karrierebibel.de/erfolg-sprueche/

How To PhD: Managing Challenging Situations During Your PhD

A PhD can be full of challenges and handling those can be difficult at times. That's why for this "How to PhD" section, we have reached out to Dan Obenchain, Junior Professor at Georg-August-Universität Göttingen, Ralf Ludwig, Professor of Physical and Theoretical Chemistry at the University of Rostock, and Jovana V. Milić, Associate Professor in Materials Chemistry at University of Turku in Finland, to get their input and advice.

The yPC Editorial Team

Dan Obenchain

Which major scientific or other challenges did you face during your PhD and how did you solve them?

I think at some point we make an epiphany that our research is unique, and that is when we find the challenge. For me, it was the spin isomers of molecular hydrogen when they form complexes. In my PhD, we were making mimics of metal organic frameworks in the gas phase and then binding molecular hydrogen to them to measure the rotational spectrum. Eventually we started to ask ourselves which signals were coming from *ortho*-hydrogen and which from *para*-hydrogen. The relative abundances of *ortho* and *para* didn't match what we knew from normal, room temperature hydrogen. We couldn't explain what we saw. As a group, we reached out to metal-ligand specialists to help us understand when to expect *ortho/para* conversion and hard-core spectroscopists to understand the complexities of the allowed transitions in our spectra. It took us months to be satisfied with our results enough to publish. It was through outreach, discussion, and collaboration that we could solve the problem.

What I understood then, and what I see all the time now, is that discussion is important, especially when we don't know the answer, or we have negative results. When I think a project might be a bit more routine than others, it never hurts to discuss the results out loud or in a short presentation. It doesn't always have to be with external collaborators, often just having more eyes on the problem will help. One person asking one question on a project might be the trick that makes it all make sense.

What advice do you give your students to manage difficult situations during their PhD?

In difficulties with my research, I always find that a bit of productivity goes a long way. Some days and some weeks feel completely unproductive. Achieving even a few small tasks daily or weekly will help to circumvent feeling unproductive in the face of a challenging research problem. At least when I leave the lab at the end of the day, I can look back and say that I did something.

In a PhD, we find that personal conflicts can arise from disagreements over results to mismanagement of resources. Most PhDs are on a timeline, finishing in an X-year timeline can add stress to any situation. Always try to remember that we all feel overwhelmed and stressed from time to time.

For either my interpersonal or my scientific issues, I recommend that everyone have someone outside of their field with whom they can discuss things. It is sometimes helpful to go over the difficulties or complain about one's own research to an outsider. As an example, I struggle with imposter syndrome. Yet, I find that many of my colleagues, especially here in Germany, don't have a clue about this difficulty. A friend outside my field or outside of research will often be able to listen and just point out the simple basics; I didn't get to my current position by being inadequate, I just felt inadequate in that moment.

When and how should students approach their supervisors with problems they cannot overcome by themselves?

In September 2024, I attended a joint workshop between two research training groups (RTGs). We had great scientific discussions, but we also made some time to discuss how each RTG was performing. One of the topics that we spent a long time discussing was student management. For this discussion, we had a group of PhD advisors from junior groups, more experienced group leaders, and PhD students at different times in their studies. What I took from this discussion was communicating early with your supervisor (or your advisory committee) about how you and your supervisor should work together. Set the expectations clearly, and stick to them as best as you can. This includes when a PhD student should be approaching their supervisor with problems. I encourage my students to have a clear understanding of the following points:

- How hard does a problem have to be before the PhD student seeks out help?
- How many solutions should the PhD student try first?
- Where to search for the answers?
- Is there someone else who you can discuss it with as an alternative in case you are unsure about approaching the supervisor?

Each PhD student has a preferred learning style that is best for them, but also each supervisor will have a management style that they find more efficient and beneficial. In a large PhD group,

there might be students that want a highly regulated PhD and others who prefer the laissez-faire approach. Some supervisors will be more open to frequent discussions and others will be more distant. This can create stress for both supervisors and students. In my opinion, we can avoid some stress and headaches by discussing early on what the expectations are.

I want my students to feel like I am approachable. When they have questions, I will always try to make time. Occasionally, there isn't enough time to discuss scientific problems. Occasionally, I find the personal problems a bit too personal. I can't say I have a perfect system, and I don't think any PhD/supervisor relationship will be perfect. As my PhD students go through their program, the expectations might need to be changed. Again, this works best with a proper discussion.

J. Prof. Dr. Daniel Obenchain

Daniel Obenchain started his research career developing instrumentation for rotational spectroscopy at Eastern Illinois University, where he received his bachelor's degree in chemistry. He continued in the field of rotational spectroscopy during his PhD at Wesleyan University, where he spent time examining the binding of molecular hydrogen to coinage metals. He was awarded an Alexander von Humboldt Postdoc Fellowship at Leibniz University Hannover in 2016. In 2018, he moved from Hannover to Hamburg to work in the rotational spectroscopy group at DESY. Since 2020, he has been building a rotational spectroscopy group (GöRotor Group) at Georg-August University Göttingen as a Junior Professor. Dan Obenchain's research focuses on benchmarking weakly bound complexes against other experiments and theory, as well as instructional methods for teaching high-resolution spectroscopy.

Ralf Ludwig

Which major scientific or other challenges did you face during your PhD and how did you solve them?

I faced two major challenges during my doctorate. The scientific challenge: I had to determine the OH reorientation times of alcohols using NMR relaxation time measurements. What sounds effortless cost me a year of synthesis work. Because of the rapid proton exchange, I had to resort to the so-called ^{17}O method. For this, I needed four differently ^{17}O-labeled alcohols, with $H_2{}^{17}O$ as the starting substance. It was simply a matter of turning water into wine. Expectedly not an easy task. But that was not enough! In order to suppress the proton interaction, the alkyl groups had to be deuterated, so deuterated methyl and ethyl iodide came into play. Nasty stuff! As a trained physicist with a two-week chemistry internship and having passed my intermediate diploma exam, I was able to rely on my (school) friends from chemistry. The synthesis steps were first noted down on a beer mat in a pub in Aachen. Like dissolves with like. $H_2{}^{17}O$ water for a total of 40,000 Deutschmarks, an autoclave and a lot of luck led to success. Now the NMR measurements could begin. "Aspect 2000" was the name of the computer in the NMR spectrometer, which liked to shut down shortly before the end of the measurement, drove me crazy, and cost me many nights. The second challenge was not of a scientific nature: while I was doing my doctorate from 1988 to 1991, I was deputy national chairman of the Young Socialists in the SPD. "100 ecological projects", 'fan projects' and 'new drug policy' took their toll. The first evaluations of my NMR experiments took place in an attic in Magdeburg. I spent about a month in Saxony-Anhalt to found local SPD associations with my friends there and to support my party's campaign for the first free parliamentary elections in Germany on December 2, 1990. My NMR measurements were more successful. The election was lost roundly. Election winner Kohl promised the "spiritual, cultural, economic and social unity of Germany" as well as a rapid equalization of living conditions for the people in the old and new federal states. We are still waiting for it. Things went much better with my doctorate. Back in Aachen, I finished my evaluations. In March, I successfully ran for the Juso national chairmanship in Potsdam. After the press conference, I had six weeks to write my dissertation, deadline April 26, defense in July, done.

What advice would you give your students to manage difficult situations during their PhD?

There are plenty of difficult situations during a doctorate. What helps a lot is: talk a lot and exchange ideas with friends and confidants, people from your own or neighboring groups, don't dig yourself in and try to deal with the problem alone. Secondly, you need a plan, not a five-year plan, but rather an announced three-year plan, with the possibility of extension. What should be done in what time? Build in a buffer for failure. Don't give up at the first hurdle. The goal can also be achieved with a little more time. Science as a whole needs more time if it is to be good, and so does a doctorate. Be self-confident about tasks in

basic research. Not every doctorate is a major step forward for mankind, but there are also no “unimportant questions” or “insignificant results”. Every small insight helps and prepares the way for bigger ones. When there is no way out: In consultation with your supervisor, take some time out to recharge your batteries. Ask to be sent to conferences and workshops. There you will meet like-minded people and scientists with similar questions and interests. The doctoral students in our group benefit from attending workshops and conferences and return highly motivated from scientific trips.

When and how should students approach their supervisors with problems they cannot overcome by themselves?

Today, a supervisor should always have an open ear and time. The door should be open. I wouldn‘t put up with scheduled appointments in two or three months‘ time. Talk to your supervisors as early as possible, not only to share successes, but especially to discuss problems. In either case you should be well prepared. If a working group is really well supervised, many problems can be solved within the group before they have to be made public.

I used to be against cumulative doctorates because important results were not properly documented. I have since changed my mind. Publications in the course of the doctorate describe milestones and give self-confidence. In the cumulative doctorate, the results are then summarized and placed in a comprehensible and convincing context. Doctorates lasting longer than five years should be a rarity.

Always take up the cudgels for basic research. Please don‘t feel guilty if you can‘t answer the question about the application potential. I was recently asked at a conference why we do the research presented here at all. The answer was short and sweet: because we want to know.

Prof. Dr. Ralf Ludwig

Ralf Ludwig was appointed Professor of Physical and Theoretical Chemistry at the University of Rostock in 2004. He has headed the Department of Physical Chemistry there since 2012. His main scientific activities are in the field of clusters, liquids and solutions.

Jovana V. Milić

Which major scientific or other challenges did you face during your PhD and how did you solve them?

One of the most critical challenges I faced during my PhD in the Department of Chemistry and Applied Biosciences at ETH Zurich in Switzerland (2013–2017) relates to pursuing a new generation of prospective molecular machines, photoredox-switchable grippers. These redox-active systems were inspired by the interactions in the photosynthetic reaction center, and they were envisaged to expand and contract in response to electric or electromagnetic stimuli, reversibly encapsulating other molecules, thereby enabling their prospective application in nanorobotics. However, this required relying on hydrogen bonding with semiquinone radical anions to trigger the switching process upon (photo)reduction of quinone species, necessitating a combined methodological approach to demonstrate the concept. It was unclear whether the lifetime of the radical species would be sufficient to assess “molecular gripping,” whereas the appropriate methods to analyze the active species were either unclear or unavailable to me at the time, making the success of the approach highly uncertain even if I managed to access the target molecular systems. Nonetheless, the prospect of the innovative molecular switching concept was very stimulating, and I managed to convince my late PhD advisor, Prof. François Diederich, that this approach would be worth pursuing, and I was privileged and honored by his support. For this purpose, I learned to model target molecular systems to theoretically assess the appropriate geometries before undertaking a complex synthetic challenge. Moreover, I contacted one of the experts on the photochemistry of semiquinone radical anions and their hydrogen bonding, Prof. Oliver Wenger, who later became a close collaborator and my PhD examiner, and who had just moved to the University of Basel at the time when I was doing my internship at the F. Hoffmann-La Roche before starting my PhD work. He kindly agreed to meet me to discuss the idea of developing a quinone-based molecular gripper to assess the feasibility of the approach. With more confidence in the concept, I proceeded to synthesize the target molecules and the corresponding model systems, and throughout this endeavor, I was fortunate to exchange with my master’s thesis adviser, Dr. Igor Pochorovski (now Lab Head at Covestro in Germany), who encouraged me to persist. With the series of desired molecular systems in hand, I contacted experts in the relevant EPR spectroscopy and spectroelectrochemistry techniques, some of whom worked on studying semiquinones in the photosynthetic reaction center of biological systems. For instance, this was Prof. Wolfgang Lubitz at the Max Planck Institute for Chemical Energy Conversion in Germany, who kindly invited me to present my preliminary work to his team and shared my enthusiasm for applying these bioinspired concepts to molecular machinery. I thereby established a collaboration with his team through one of the senior researchers, now long standing collaborator, Dr. Michal Zalibera, who introduced me to other colleagues working on related EPR methods in the group of Prof. Georg Gescheidt at the Technical University of Graz in Austria, as well as UV-vis spectroelectrochemistry at the Institute Le Bel of the University of Strasbourg in France with Prof. Laurent Ruhlmann and Prof. Corinne Boudon, initiating a lasting collaboration that shaped my development as a scientist. This ultimately resulted in

successfully demonstrating the desired molecular gripper behavior with unique control by electrical or electromagnetic stimuli of interest to the scientific community [1–4]. The work was published in 10 articles over a five-year period between 2014 and 2019, and I was invited to present it at the Molecular Machines Nobel Prize Conference at the University of Groningen in 2017. Moreover, I was awarded the Helvetica Prize in 2018/2019 for the best-selected publication by a young researcher in Switzerland [2]. More importantly, this experience left a lasting mark on my academic career and development as a researcher and scholar, teaching me a valuable lesson on perseverance in the face of adversity when driven by scientific curiosity, as well as the importance of cross-disciplinary collaboration in addressing complex challenges, which I nurture in my independent academic career [5].

What advice would you give your students to manage difficult situations during their PhD?

I hesitate to offer general advice to students in managing difficult situations during their PhD, as each experience is unique. With that in mind, the only appropriate advice I would permit myself to offer is to embrace this uniqueness with authenticity, recognizing it as a powerful resource, especially in the face of challenges. We all have our own journeys, which cannot be compared to anyone else's. Once we accept this reality and recognize our intrinsic values, motivations, and drives, the "difficult situations" cease to exist as they become only steps on the way to realizing our path with purpose and joy.

When and how should students approach their supervisors with problems they cannot overcome by themselves?

This question reminds me that traditional academic training often assumes that young scientists need to learn how to "solve problems and overcome them by themselves." There is some truth to the importance of such research independence, building confidence and the capacity to tackle complex scientific questions. However, this often comes at the expense of recognizing that, in the real world, scientists do not operate individually. The images of a "lonely genius" can be very misleading, creating conflicting expectations for young scientists about their role in science, research, and broader society. Some of the most complex contemporary challenges require extensive teamwork across the boundaries of disciplines. Recognizing this points to the criticality of raising scientists who can effectively work and communicate in a team. This is also relevant when it comes to addressing the question of when and how to approach supervisors or co-workers with problems that cannot be overcome individually. I believe that science should involve a shared pursuit of knowledge and discovery, which does not only involve conventional research but also continuous discussion and exchange about the scientific questions, hypotheses, and methodology to address them, as well as expectations in the process. With that in mind, the students should be provided with an environment in which they can openly express their concerns and share problems and ideas of prospective solutions, as this contributes to their development as scientists, researchers, and independent thinkers, as well as critical problem-solvers, who do not hesitate to recognize issues and express them so that they can engage in the pursuit of knowledge, curiosity, and discovery freely without unnecessary obstacles of formality or communication barriers. Of course, this should also be discussed with the respective supervisors to align expectations early on. I hope such an approach could ensure a more productive environment for personal and professional growth while nurturing awareness for a more meaningful contribution to broader society.

References

[1] J. V. Milić, F. Diederich, 'The Quest for Molecular Grippers: Photo-Electric Control of Molecular Gripping Machinery', *Chem. – Eur. J.* 2019, **25**, 8440–8452.

[2] J. V. Milić, T. Schneeberger, M. Zalibera, K. Z. Milowska, Q. K. Ong, N. Trapp, L. Ruhlmann, C. Boudon, C. Thilgen, F. Diederich, 'Thioether-Functionalized Quinone-Based Resorcin[4]arene Cavitands: Electroswitchable Molecular Actuators', *Helv. Chim. Acta* 2019, 102, hlca.201800225.

[3] J. Milic, M. Zalibera, D. Talaat, J. Nomrowski, N. Trapp, L. Ruhlmann, C. Boudon, O. S. Wenger, A. Savitsky, W. Lubitz, F. Diederich, 'Photoredox-Switchable Resorcin[4]arene Cavitands: RadicalControl of Molecular Gripping Machinery via Hydrogen Bonding', *Chem. – Eur. J.* 2017, **23**, 1431–1440.

[4] J. V. Milić, M. Zalibera, I. Pochorovski, N. Trapp, J. Nomrowski, D. Neshchadin, L. Ruhlmann, C. Boudon, O. S. Wenger, A. Savitsky, W. Lubitz, G. Gescheidt, F. Diederich, 'Paramagnetic Molecular Grippers: The Elements of Six-State Redox Switches', *J. Phys. Chem. Lett.* 2016, **7**, 2470–2477.

[5] www.jovanamilic.com (Accessed on Dec 5, 2024)

Ass. Prof. Dr. Jovana V. Milić

Jovana V. Milić is appointed Associate Professor in Materials Chemistry at the University of Turku in Finland in September 2024. She has been an Assistant Professor and Group Leader at the Adolphe Merkle Institute of the University of Fribourg in Switzerland since September 2020, leading the Smart Energy Materials team as a Swiss National Science Foundation PRIMA Fellow. She conducted her postdoctoral research at the Laboratory of Photonics and Interfaces at EPFL between 2017 and 2020, after she obtained her PhD in Chemistry at ETH Zurich in Switzerland in 2017. Her research is focused on developing hybrid stimuli-responsive (supra) molecular materials for sustainable energy conversion, with a particular focus on photovoltaics. In addition to interdisciplinary research and international collaborations, as a member of the Swiss and Global Young Academies and the International Science Council Fellow, she has been invested in connecting and supporting young scientists at the interface of science, policy, and diplomacy toward sustainable development worldwide.

How To Adjust to New Working Environments

Navigating new working environments is a crucial skill for any researcher, especially during a PhD, where cultural and professional transitions often go hand in hand. In this section, we bring you two insightful contributions that explore this dynamic in depth. The first article, *"International Communication and Culture in STEM,"* delves into the nuances of cross-cultural communication, offering valuable tips on how to bridge cultural gaps and thrive in a globally interconnected field. Complementing this, we present a collection of four short reports and interviews with international students who have experienced moving to, from, or between countries – including Germany – and share how these transitions have shaped their personal and professional growth. Together, these articles aim to provide you with actionable insights to better prepare for and adapt to new working environments, helping you make informed decisions as you chart your own PhD journey.

The yPC Editorial Team

Charlotte Gerischer

International Communication and Culture in STEM

The principle of research is based on continuous exchange of knowledge. We conduct research based on data collected by others and benefit from their expertise to develop our own hypotheses. But not only is expertise important, also everything around it. Someone who studied in Munich has, in broad terms, studied the same subjects as a student from Hamburg, but in detail they will have learned different tips, tricks and approaches. The same holds true for international education.

Everywhere, the focus is different, and knowledge is conveyed in different ways. This diversity in educational methods is one of the key reasons why international exchange is so valuable. Science has embraced international collaboration, and its neutral, objective nature helps overcome barriers that other fields still struggle with.

However, international students face problems and challenges during their studies abroad. These challenges usually do not root in the absence of skill but one thing that unfortunately often is overlooked in the STEM Community – **Culture and Communication**.

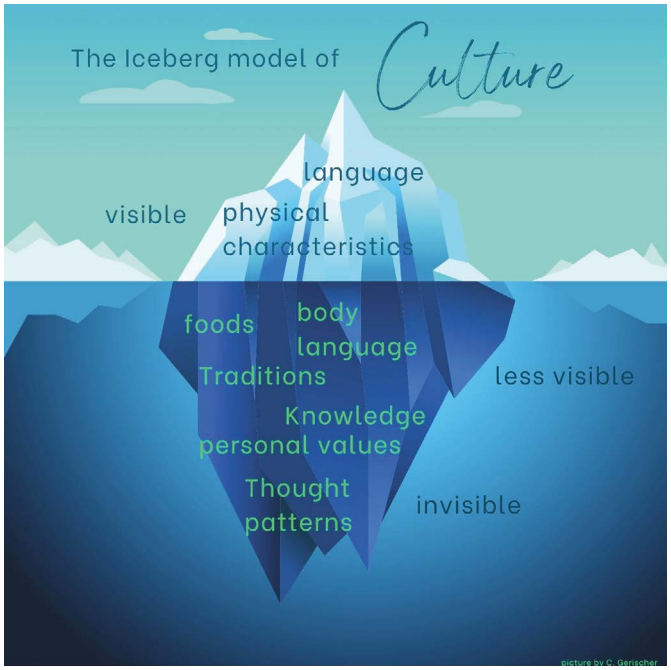
Cultural differences significantly impact the dynamics of work in a laboratory. International students already are challenged in social integration because of language barriers and the absence of an established social network. This can lead to feelings of isolation which can negatively impact mental well-being and academic performance. During the first months abroad, work often becomes a social center. Therefore colleagues and the PI should be aware of the additional effort required for integration.

The language barrier only poses one of the communicational problems in the beginning. Scientific communication can be hindered by unfamiliar terms or inaccurate wording. In addition, laboratories often have unwritten rules and cultural expectations that newcomers may not understand. These rules can include initiative, responsibility or ways of collaboration. For example, in some cultures, students are expected to work autonomously, while in others, a more defined hierarchy exists with clear task assignments. International students must learn to recognize these unwritten rules and navigate their new working environment, even though they are often not explicitly taught.

To understand these problematics and their potential to conflict better, it is important to understand the concept of culture and its impact on communication.

A useful framework for understanding our perception of Culture is the **Iceberg Model** by E.T. Hall. According to this model, only 10% of culture is visible – through things like language, food, and clothing – while the remaining 90% is hidden beneath the surface, shaped by deeper values, beliefs, and social norms. When moving to a new country, international students initially interact with only the visible part of the culture, and it takes time to understand the hidden aspects.

Charlotte Gerischer
Team Podcast und Team Chancengleichheit
JungesChemieForum (JCF) der Gesellschaft Deutscher Chemiker (GDCh)
c.gerischer@jcf.io



The Iceberg Model of Culture. (Copyright: Charlotte Gerischer)

Different countries, for example, vary in their communication style. While Germany has a "low-context" communication, where words directly convey their meaning and body language and facial expression are rather unimportant, France has a "high-context" communication that places more importance on body language and emotional nuance. A French person might interpret a German's blunt directness as rude and uninvested, while the German might find the French person's indirectness confusing or even insincere.

Both were in the same situation and yet each of them experienced a completely different one.

These differences are not just present in everyday communication but also affect academic settings. In many countries, students are encouraged to address professors directly, while in others, there is more emphasis on hierarchy and formal, reserved communication. Students in these cultures may show respect through restraint and less direct confrontation with their supervisors.

The key to overcoming these challenges apart from understanding their source is openness and patience. Both international students and local colleagues must understand that misunderstandings often arise from differing cultural perceptions of the same situation. Recognizing these differences can help prevent conflicts and facilitate better collaboration.

It is therefore crucial that everyone actively participates in integration efforts. Some institutions have already developed successful programs to facilitate the transition for foreign students. Orientation programs, intercultural workshops, and mentoring schemes can help speed up the integration process. Likewise, international networks regularly offer events and workshops.

Practical suggestions for improving inclusion include providing language support for international students and organizing regular team events to encourage exchange through peer-mentoring programs. Such measures contribute to strengthening the sense of belonging and are promoting social integration. And if everyone steps a bit further towards their counterpart, the magic of a deeper understanding will happen.

Charlotte Gerischer

Charlotte Gerischer (she/her) is studying chemistry at TU Berlin in Germany and is currently finishing her masters in bioorganic catalysis. Outside of her studies, Gerischer is widely engaged in multiple associations and has a wide range of interests. She works as a volunteer in the GDCh (German Chemical Society), where she has been leading the Team Equal Opportunities for several years. This team focuses on the representation of marginalized groups, the prevention of all forms of discrimination, and the promotion of equality of opportunity within the GDCh and the field of chemistry. For the past 13 years, she has also been active in Experiment e.V., an association that promotes intercultural friendship and exchange. As part of her engagement she gives lectures and workshops on intercultural communication and has participated in various professional development programs.

Your Publications: Communicated!

A new category has recently been added to the Bunsen-Magazin, "Your Publications: Communicated!", where young scientists present their scientific publications in a short article to the readers of the Bunsen-Magazin.

If you want to be featured as well, submit your short contribution consisting of an abstract and a figure to yPC@go.bunsen.de, and we will select the best contributions to be published in one of the next Bunsen-Magazin issues. The length of the submission, excluding the figure, should not exceed half a page (around 700 characters), and the figure should illustrate the presented research. The publications must have been published less than two years ago in a peer-reviewed journal. We welcome contributions from young researchers in all career stages up to two years after their PhD defence, who have contributed significantly to the presented publication. In case of a shared first authorship, we also accept shared submissions from the authors with equal contributions.

We look forward to your contributions!

Noah and Katharina
(yPC speakers)

Short Reports of International Students

My decision to study abroad:

I decided to pursue my graduate studies outside of Germany to challenge myself. Navigating life in a new country while adapting to a second language pushes us out of our comfort zone, allowing us to learn more about ourselves and expand our boundaries. It enables us to experience other cultures, giving us a view of life from a different angle. Additionally, it is a unique opportunity to build friendships with people from around the world.

Benefits and challenges of doing a PhD abroad:

A PhD in the UK places a stronger emphasis on a structured, student-centered learning experience. Unlike the German system, where a PhD candidate is often treated more like an employee, in the UK the emphasis is more pedagogical, with clearer milestones to support progress. This shift comes with benefits and challenges: Without a default salary as in Germany, securing a stipend became essential. Additionally, moving to an entirely new academic environment required me to build a fresh network of contacts and support, which was quite different from the familiar setting at my undergraduate university in Bonn.

Lorenz Omran

University of Oxford
lorenz.omran@chem.ox.ac.uk

Useful links if you consider studying in the UK

www.rsc.org/careers

www.findaphd.com

www.jobs.ac.uk

https://www.findaphd.com/funding/guides/phd-funding-guide.aspx

https://www.findaphd.com/funding/guides/international-phd-funding-uk.aspx

https://www.findaphd.com/advice/blog/6288/international-phd-students-to-be-eligible-for-research-council-studentships-in-2021-22

https://www.findaphd.com/funding/guides/epsrc-funding.aspx

Why I decided to pursue graduate studies in Germany:

My name is Weishan Wu, from China. After completing my bachelor's degree in materials engineering, I decided it was time for an adventure abroad. A childhood friend of mine had moved to Germany many years earlier to study piano, and she often shared stories about her life there – how fascinating the different lifestyles are, and the unique way of life in Germany. Plus, ever since I was in school, I'd read about so many famous German scientists in my physics and chemistry textbooks! All of these influences, along with Germany's reputation for scientific excellence, particularly in scientific research and engineering, sparked my interest and curiosity about studying and living in Germany myself. Looking back, it was one of the best decisions I've ever made. This journey has given me the chance to immerse myself in a completely new world, engage with people from diverse backgrounds, learn the German language (a challenge in itself!), and experience the country's history and vibrant traditions. These experiences haven't just enriched my personal development but also broadened my academic skills. The program offered by Philipps University Marburg was a wonderful place to dive deeper into materials science. I'm so inspired that I've decided to keep going and pursue a doctorate degree, to the next chapter of the adventure!

Benefits and challenges of pursuing a PhD in Germany:

I am currently in my second year of a PhD in electrochemical 3D printing at Carl von Ossietzky University. The university has provided numerous benefits, including access to cutting-edge research facilities and generous funding opportunities, which have made my research possible. My supervisor offers a high level of guidance and support, and my colleagues are highly skilled, with strong backgrounds in their fields. They are always willing to help, creating a collaborative and encouraging environment. However, the challenges are significant. Researching at the edge of human knowledge often feels like a vast endeavor, where there's always more to learn and explore, never enough! Balancing this constant drive for knowledge with maintaining a work-life balance has been one of the toughest parts of the journey. However, dealing with the stress and disappointment when research doesn't go as expected is also part of the scientific process; overcoming these moments brings personal growth and a resilience that makes the journey worthwhile!

Weishan Wu

Carl von Ossietzky Universität
Oldenburg
weishan.wu@uni-oldenburg.de

Doing a Joint PhD - what's that?

"The Joint PhD programmes are conducted on a full-time basis. Students in the programmes are registered at both NTU and the partner university. Upon successful completion of the programme, NTU and the partner university will jointly confer the PhD degree." This rather unromantic statement is how my home institution, the Nanyang Technological University Singapore, describes to the point what a joint PhD is all about. After starting my PhD studies at NTU in the School of Materials Science and Engineering in 2022 and completing my qualifying exam, I was able to switch to a joint programme and have been at the Department of Chemistry at the University of Warwick since February 2024. Spending a minimum of 1 year in the UK, I am able to increase my network globally, and combine the application-oriented knowledge I obtained in Singapore with some of the unique methods available only in my research group in Warwick. This type of opportunity also exists for many German programmes collaborating with schools overseas, as long as they have an ongoing agreement for it. No matter if you are looking for a place to start your PhD or if you want to "upgrade" your programme in the middle of doing it - be on the lookout for joint schemes like this, as they are oftentimes just a bit out of sight when not explicitly looking for them!

Caught between three worlds - challenges of pursuing a PhD in Singapore and the UK as a German:

Of course, being in such an international programme with ongoing collaborations in Germany comes with its own unique challenges. Balancing three different time zones for regular meetings, constantly traveling (and consequently "living out of a suitcase"), and having an English accent that becomes an illegible amalgam of the idioms and cultures of the people you encounter during your international endeavors are definitely some of the things you should be prepared for. However, personally, I wouldn't want to have it any other way. If you are passionate about research, exchanging ideas on a global scale, and don't mind longer plane and coach rides, I encourage everyone to have a good think and consider an opportunity like this for themselves.

Noah Al-Shamery

Nanyang Technological University
Singapore/University of Warwick
noahcoel001@e.ntu.edu.sg
Noah.Al-Shamery@warwick.ac.uk

What is your background?

I graduated with an MSc in chemical engineering from Budapest in 2021. After gaining industrial experience at Sanofi and MSD Animal Health, I decided to pursue a PhD in chemistry at the University of Vienna. My goal in returning to academia was not only to enhance my career prospects but also to learn the German language.

Why did you choose to do your PhD in Austria?

The country itself wasn't a primary factor for me. However, Austria has the advantage of proximity to my home in Hungary, allowing me to visit my family on weekends. Additionally, since I had already been living in Austria for almost a year before starting my PhD, I didn't need to relocate. This continuity made the transition to academic life easier.

What are the benefits and challenges of doing your PhD in Austria, and do you like it?

There are many benefits to pursuing a PhD in Austria, especially with the University of Vienna's excellent resources and strong support for scientific research. I appreciate the autonomy that comes with academic work; it allows me to deeply explore and develop my own ideas. This is quite different from my experience in industry, where teamwork and collaborative efforts drive projects to success. In academia, however, PhD research often requires working independently, almost like a "lone wolf." I find the balance challenging yet rewarding, as it pushes me to develop self-reliance and a new level of discipline. Additionally, the PhD journey has improved my soft skills, particularly in communicating complex topics to a broader audience. This skill is invaluable, as it ensures research can reach and resonate with people beyond the scientific community. Overall, I am finding the experience both professionally and personally fulfilling.

How did you adapt to cultural differences in the working and social cultures of Austria and Hungary?

The cultural differences between Austria and Hungary are not particularly pronounced. Both countries share similar historical and cultural backgrounds, making the adjustment smoother.

Anonymous contribution

Maren Podewitz

In Computational Search of Better Catalysts

Intro

Catalysts enable the selective activation of inert chemical bonds, often under mild conditions, by lowering the activation energy of reactions. They are vital to the chemical industry, where approximately 85% of all processes rely on catalysts. Moreover, their energy and atom efficiency position them as a cornerstone of green chemistry. While heterogeneous catalysts dominate industrial applications, homogeneous catalysts offer precise control over the ligand environment, enabling fine-tuning of their properties. Improving their performance is therefore of utmost importance from an economical and environmental point of view. Computational chemistry has been instrumental in uncovering structure-function relationships, providing insights that guide experimental development. However, predictive accuracy remains limited, primarily because computational models often fail to replicate the experimental conditions under which catalysts operate. To address this, my research group focuses on developing multiscale operando models, bridging the gap between experimental observations and computational predictions. This approach aims to improve the predictive power of computational studies, facilitating the design of more efficient catalysts.

Transition-metal complexes are central to the development of new catalysts for efficient chemical transformations due to their high selectivity and diverse coordination geometries, which allow precise tuning of properties. Rational catalyst design is driven by advances in experimental and analytical techniques, as well as theoretical and computational chemistry, which help to characterize reactive species, intermediates and products. Computational chemistry, in particular, facilitates the discovery of novel reactivities, elucidates mechanistic pathways, and accelerates the transition from discovery to optimization by guiding experimental efforts [1, 2].

While there has been significant progress in *in situ* and *operando* spectroscopy, time-resolved single-molecule studies remain challenging due to the difficulty of detecting low-concentration species with the required spatial and temporal resolution.[3] Computational methods fill this gap by providing detailed temporal and spatial insights into atomistic processes. They uniquely identify transient species, explore molecular transformations, provide insights into the thermodynamics and kinetics of chemical reactions, and thus aid in the design and optimization of chemical processes [4, 5].

The ultimate goal is to predict stable, selective and active catalysts using computational methods. This can be approached through a “chemical” strategy that focuses on accurately describing the reaction mechanism [4], or through a data-driven approach that uses statistical models and machine learning to analyze experimental or computational data [5]. In both cases, the accuracy of the predictions depends critically on the precision of the calculations. To achieve the highest possible accuracy in the calculations and to derive reliable predictions, it is essential to model the catalyst as realistically as possible [6].

This process involves selecting an appropriate computational method and constructing a realistic chemical model (see Figure 1). The computational method determines the level of theory used to describe the system and is chosen based on the size and nature of the molecule and the question being addressed. For example, electronic structure methods are essential for studying changes in covalent bonding, whereas molecular mechanics models are sufficient to describe non-covalent interactions. The chemical model incorporates, at the bare minimum, the molecular structure of the compound under study. Ideally, the results obtained should be compared with reference data. If there are discrepancies, the calculation method is usually refined, for example, by using a more advanced density functional or switching to wave function theory. However, the chemical model itself is often overlooked, despite its significant impact. Factors, such as explicit solvent molecules, counter ions, conformational flexibility and dynamic effects, can drastically alter reaction mechanisms and reactivities, often contributing larger errors than the calculation method itself [7]. While a full *ab initio* description accounting for all environmental and dynamic effects at the quantum chemical level would be ideal, it remains computationally infeasible for most catalytic systems. To address this, we develop tailored approaches that progressively incorporate environmental effects, balancing accuracy and feasibility for the system and questions at hand.

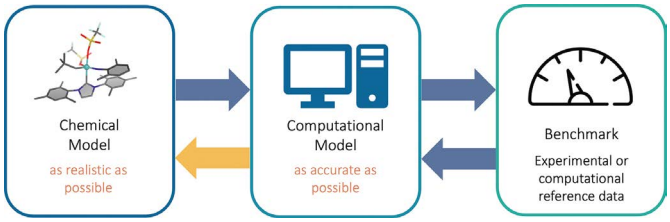


Fig. 1: Computational chemistry workflow, selecting a chemical and a computational model, comparing with reference data and adjusting both the computational and chemical model in case of discrepancies.

Prof. Dr. Maren Podewitz
Institut für Materialchemie
TU Wien
Getreidemarkt 9, AT 1060 Wien
Maren.podewitz@tuwien.ac.at
www.podewitz-lab.org

Modelling reaction mechanisms

Olefin metathesis is a fundamental reaction in chemistry, enabling the redistribution of alkene fragments, and is one of the few examples of homogeneous catalysis used on an industrial scale [8, 9]. Its success can attributed to the development of highly efficient Ru- or Mo-based catalysts [10, 11]. A significant recent milestone was the creation of a highly active, functional group tolerant Mo imido alkylidene N-heterocyclic carbene catalyst (Figure 2 (left)) [12]. To facilitate large-scale applications, understanding the activation mechanism of these catalysts to form the active species is crucial. Our DFT calculations revealed that the reaction proceeds via a previously unreported neutral olefin adduct, followed by cycloaddition and cycloreversion steps to yield the final product (Figure 2 (right)) [13]. Modeling the free energy profile required incorporating the dissociated triflate ion and treating the catalyst:triflate pair as a supramolecular complex. This approach took into account the electrostatic stabilization of triflate, which outweighed the associated entropic penalties. To explain the *E*-selectivity of the same catalyst with norbornene, where four stereoselective reaction pathways are possible, various reaction pathways were investigated [14]. Extensive conformer searches were essential to identify the most stable products. Using the Conformer-Rotamer Ensemble Sampling Tool (CREST) [15] to generate an initial conformer ensemble, followed by clustering and reoptimization with DFT [16], we identified structures that were up to 40 kJ/mol more stable than those predicted by chemical intuition [14]. By combining these techniques, we were able to show that for one of the four stereoselective pathways, a different reaction pathway became accessible, explaining the experimentally determined *E*-selectivity [14].

Conformations in explicit solvent

To improve chemical models, it is essential to explore catalyst conformers not only in implicit but also in explicit solvent. This is particularly important for large and flexible complexes, where explicit solvent molecules prevent unrealistic compact structures with many intramolecular H-bonds or the collapse of molecular cavities [21]. While existing methods for exploring conformations in explicit solvent often specifically target biomolecules, molecular dynamics (MD) simulations offer a more general approach. By simulating the system in explicit solvent and clustering the resulting trajectories, frequently visited conformations representing energy minima can be identified [22]. However, running MD simulations requires force fields, and parameterizing (transition-) metal-containing systems can be complex and time-consuming. To simplify this process, we developed PyConSolv, an open-source Python package designed to automate the generation of conformers for metal- and nonmetal-containing complexes in explicit solvents using classical MD simulations [23]. PyConSolv is an all-in-one tool for the generation of conformers in any solvent. Input requirements are minimal; only the geometry of the structure and the desired solvent in xyz (XMOL format) are required. It not only streamlines the workflow but also interfaces with popular computational chemistry software, offering a user-friendly tool for solvent-specific conformer generation.

Microsolvation models

Explicit solvent interactions affect not only the accessible conformer space, but also the efficiency of many chemical reactions. While implicit solvent models provide a simple and

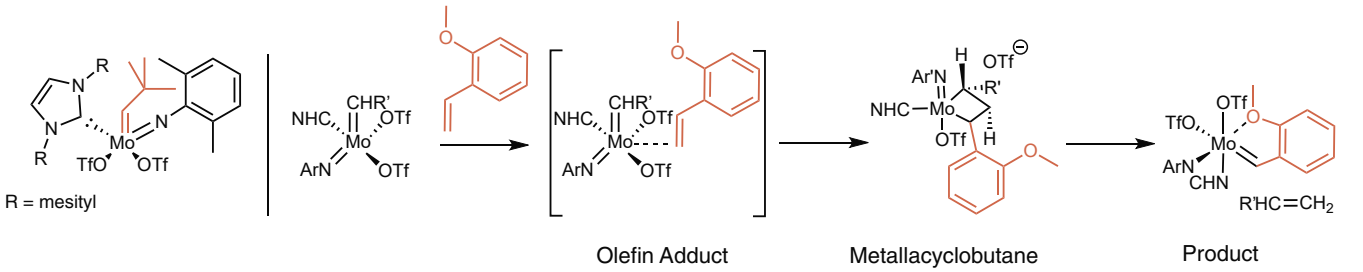


Fig. 2: Left: Mo imido alkylidene N-heterocyclic carbene catalyst. Right: Mechanism of olefin metathesis including adduct formation, cycloaddition to form the metallacyclobutane and cycloreversion to form the product.

Recent efforts to develop more environmentally benign catalysts for olefin metathesis have focused on exploring Fe-based compounds. These systems were initially studied computationally, with some viable catalysts later being successfully developed and tested experimentally [17-19]. However, despite the significant role of Mn(I) in homogeneous catalysis and its diagonal relationship to Ru(II), the potential of Mn(I)-based catalysts for olefin metathesis remains largely unexplored. As computational chemistry allows the assessment of chemical reactivity prior to experimental realisation, this prompted us to investigate the viability of Mn(I) species for olefin metathesis. Our results suggest that Mn(I) could be a promising catalyst for this reaction, although a careful balance of ligands is required to achieve a functional system [20].

cost-effective approach, they fail to capture the nuances of explicit solute-solvent interactions that affect reactivity and selectivity [24]. Full condensed-phase treatments [25], which consider both solute and solvent quantum mechanically, offer the highest accuracy but are computationally expensive and limited to small systems. A more practical alternative is the use of implicit-explicit hybrid methods, such as cluster or microsolvation approaches, which include a small number of explicit solvent molecules in quantum chemical calculations while the rest are treated at a lower level [26-28]. However, these approaches raise challenges related to determining the number, placement, and orientation of solvent molecules.

We have addressed these challenges with our Free Energy Based Identification of Solvation Sites (FEBISS) method [29].

In FEBISS, we start with a full condensed-phase MD simulation at the molecular mechanics level, which is crucial for obtaining reliable solution conformations of the solute. Central to our method is the automated placement of individual solvent molecules based on solvation free energy thermodynamics derived from MD simulations and Grid Inhomogeneous Solvation Theory (GIST) [30]. This approach allows us to rigorously define the number, position, and orientation of solvent molecules and assess their interactions with the solute (for workflow see Figure 3). The resulting solute–solvent clusters serve as input for subsequent quantum chemical analyses, providing a more accurate representation of the system and can be applied to any molecular system as long as the speciation is known and force field parameters can be provided [29].

in explicit solvent, which allowed us to elucidate the mechanism behind the high catalytic activity of this catalyst [21]. The same protocol was applied to explain the deactivation mechanism of a regioisomeric Cu-calixarene catalyst [35].

To evaluate the effect of encapsulation on the reaction dynamics, we developed a QM/MM MD model to study the key step of C-N bond formation. In this model, the reactive center is treated quantum mechanically (see Figure 4 blue Lewis formula), while the calixarene macrocycle and the explicit solvent (chloroform) are modeled with a force field. The low barrier of the C-N coupling step allowed the reaction to occur spontaneously within 20 ns of simulation time without the need for biasing. Using the semi-empirical GFN2-xTB method [36], which shows good agreement

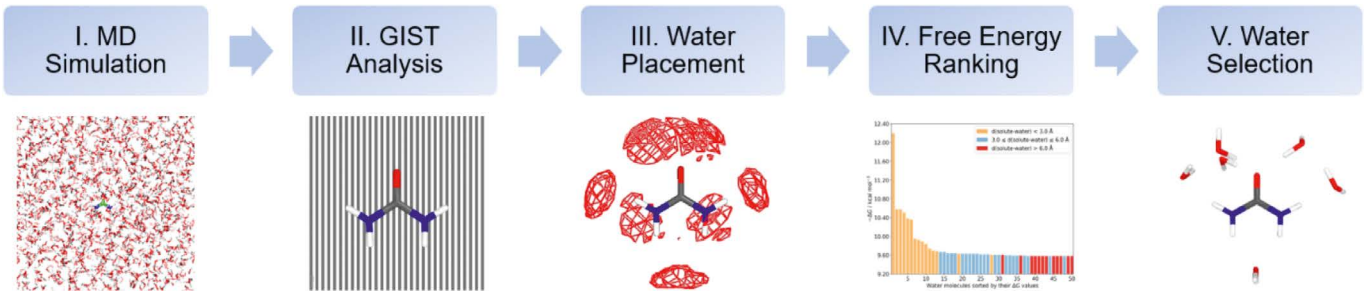


Fig. 3: FEBISS workflow to obtain microsolvation clusters: I. MD simulation of restrained solute; II. GIST analysis, III. Solvent placement based on averaged solvent density, IV. Ranking of individual solvent molecules according to their free energy: V. Selection of solvent molecules based on free energy. Reprinted with permission from Ref. [29].

Reaction Mechanisms of supramolecular catalysts/ From static to dynamic models

C-N and C-S bond formation are reactions in high demand, as amine derivatives and organosulfur compounds are key reactants for the synthesis of pharmaceuticals and high performance materials [31, 32]. The development of efficient catalysts based on earth-abundant metals, such as copper, is vital for more sustainable production processes but difficult to achieve [33, 34]. However, bio-inspired encapsulation using calix[8]arene has led to the development of functional Cu-based catalysts, [Cu1,5-(C_8PhenMe$_6$)I]], where the reactive center is a Cu-phenanthroline moiety (see Figure 4). To study the reactivity of such catalysts, we developed a multiscale workflow combining MD simulations and quantum chemical methods to account for the conformational flexibility of the macrocyclic ligand in explicit solvent. Using our PyConSolv tool, we determined realistic conformations of reactants, products, intermediates, and key transition states

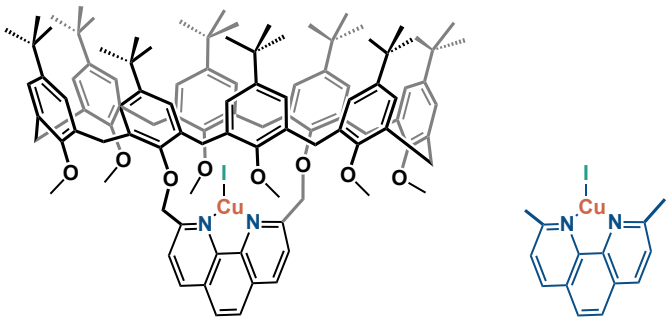


Fig. 4: Lewis formula of the supramolecular C-N coupling catalyst [Cu1,5-(C_8PhenMe$_6$)I]], as well as its reactive Cu-phenanthroline reactive center, color-coded in blue.

with DFT, we were able to repeatedly sample the reaction step, taking into account thermal and solvent fluctuations as well as conformational diversity, thus ensuring statistical accuracy [37].

Extracting chemical information from large data

To extract the reaction coordinate from over 130 simulation trajectories, we turned to statistical and machine learning (ML) techniques due to the large amount of data. We combined both supervised and unsupervised ML methods to effectively analyze the data and extract chemically relevant information.

We used the energy of the system over the simulation time to label the structures as educts, transition states or products. The reaction energy was calculated by averaging the ensembles of educt and product states. A sigmoid fit to the smoothened energy profile of each simulation allowed us to identify and calculate the energy barrier [37]. To find the reaction coordinate, we aimed to identify the minimal set of molecular features, here internal coordinates, most correlated with the energy change during the reaction. Describing the molecule with internal coordinates and removing highly correlated coordinates was necessary before applying techniques such as Principal Component Analysis and Linear Discriminant Analysis to capture the largest variations in the data. To maximize the separation between the three states (educt, transition and product) while also reducing the number of internal coordinates, we trained multiple explainable machine learning models. To minimize method dependency, a consensus model was applied to identify features that were common to at least 75% of the analyses. Granger causality analysis was then performed on the

consensus features to decompose the reaction coordinate into a series of molecular motions. This analysis clearly highlighted the peripheral contributions of the calixarene cage to the C-N coupling step [37].

The reaction coordinate was quantified using decision trees, which classify ensembles by setting cut-offs for coordinates such that the separation between different classes is maximized, starting from the coordinate that gives the best separation. However, since decision trees are sensitive to initialization, a more robust approach is random forest, which trains multiple decision trees on subsets of the data. The results of the random forest analysis can then be translated into semantic rules, allowing classification based on the quantitative values of the internal coordinates [37].

Summary

The examples from transition-metal catalysis demonstrate how tailored multiscale models can improve accuracy and deepen our understanding of catalyst functionality. The incorporation of factors such as conformational diversity in explicit solvents, counterions, and dynamic effects are key steps in the development of computational operando models that bridge the gap between theory and experiment. These advances are essential for the in silico design of improved catalysts to guide experimental research efforts.

References

[1] J. Jover and N. Fey, The Computational Road to Better Catalysts, *Chem. Asian J.*, 2014, **9**, 1714–1723.

[2] L. Mammino, Green chemistry and computational chemistry: A wealth of promising synergies, *Sustain. Chem. Pharm.*, 2023, **34**, 101151.

[3] K. Köhnke, N. Wessel, J. Esteban, J. Jin, A. J. Vorholt and W. Leitner, Operando monitoring of mechanisms and deactivation of molecular catalysts, *Green Chem.*, 2022, **24**, 1951–1972.

[4] S. Ahn, M. Hong, M. Sundararajan, D. H. Ess and M. H. Baik, Design and Optimization of Catalysts Based on Mechanistic Insights Derived from Quantum Chemical Reaction Modeling, *Chem. Rev.*, 2019, **119**, 6509–6560.

[5] A. Nandy, C. Duan, M. G. Taylor, F. Liu, A. H. Steeves and H. J. Kulik, Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning, *Chem. Rev.*, 2021, **121**, 9927–10000.

[6] O. Eisenstein, G. Ujaque and A. Lledos, in *New Directions in the Modeling of Organometallic Reactions*, eds. A. Lledos and G. Ujaque, Springer, Switzerland, 2020, vol. 1, pp. 1–38.

[7] M. Besora, A. A. C. Braga, G. Ujaque, F. Maseras and A. Lledos, The importance of conformational search: a test case on the catalytic cycle of the Suzuki-Miyaura cross-coupling, *Theor. Chem. Acc.*, 2011, **128**, 639–646.

[8] J. H. Phillips, in *Organometallic Chemistry in Industry*, John Wiley & Sons, Ltd, 2020, pp. 259–282.

[9] L. Ondi, G. M. Nagy, J. B. Czirok, A. Bucsai and G. E. Frater, From Box to Bench: Air-Stable Molybdenum Catalyst Tablets for Everyday Use in Olefin Metathesis, *Org. Process Res. Dev.*, 2016, **20**, 1709–1716.

[10] T. M. Trnka and R. H. Grubbs, The Development of L2X2Ru = CHR Olefin Metathesis Catalysts: An Organometallic Success Story, *Acc. Chem. Res.*, 2001, **34**, 18–29.

[11] R. R. Schrock, Olefin Metathesis by Molybdenum Imido Alkylidene Catalysts, *Tetrahedron*, 1999, **55**, 8141–8153.

[12] M. R. Buchmeiser, S. Sen, J. Unold and W. Frey, N-Heterocyclic Carbene, High Oxidation State Molybdenum Alkylidene Complexes: Functional-Group-Tolerant Cationic Metathesis Catalysts, *Angew. Chem. Int. Ed.*, 2014, **53**, 9384–9388.

[13] K. Herz, M. Podewitz, L. Stöhr, D. R. Wang, W. Frey, K. R. Liedl, S. Sen and M. R. Buchmeiser, Mechanism of Olefin Metathesis with Neutral and Cationic Molybdenum Imido Alkylidene N-Heterocyclic Carbene Complexes, *J. Am. Chem. Soc.*, 2019, **141**, 8264–8276.

[14] M. Podewitz, S. Sen and M. R. Buchmeiser, On the Origin of E-Selectivity in the Ring-Opening Metathesis Polymerization with Molybdenum Imido Alkylidene N-Heterocyclic Carbene Complexes, *Organometallics*, 2021, **40**, 2478–2488.

[15] P. Pracht, F. Bohle and S. Grimme, Automated Exploration of the Low-Energy Chemical Space with Fast Quantum Chemical Methods, *Phys. Chem. Chem. Phys.*, 2020, **22**, 7169–7192.

[16] M. Podewitz, in *Chemical Modelling*, 2022, vol. 37, pp. 1–23.

[17] S. Takebayashi, M. A. Iron, M. Feller, O. Rivada-Wheelaghan, G. Leitus, Y. Diskin-Posner, L. J. W. Shimon, L. Avram, R. Carmieli, S. G. Wolf, I. Cohen-Ofri, R. A. Sanguramath, R. Shenhar, M. Eisen and D. Milstein, Iron-catalysed ring-opening metathesis polymerization of olefins and mechanistic studies, *Nat. Catal.*, 2022, **5**, 494–502.

[18] Z. S. Lincoln and V. M. Iluc, Iron Olefin Metathesis: Unlocking Reactivity and Mechanistic Insights, *J. Am. Chem. Soc.*, 2024, **146**, 17595–17599.

[19] É. de Brito Sá, L. Rodríguez-Santiago, M. Sodupe and X. Solans-Monfort, Toward Olefin Metathesis with Iron Carbene Complexes: Benefits of Tridentate σ-Donating Ligands, *Organometallics*, 2016, **35**, 3914–3923.

[20] J. Pecak, R. A. Talmazan, D. Svatunek, K. Kirchner and M. Podewitz, Is Mn(I) More Promising Than Fe(II)—A Comparison of Mn vs Fe Complexes for Olefin Metathesis, *Organometallics*, 2024, **43**, 457–466.

[21] R. A. Talmazan, J. Refugio Monroy, F. del Río-Portilla, I. Castillo and M. Podewitz, Encapsulation Enhances the Catalytic Activity of C-N Coupling: Reaction Mechanism of a Cu(I)/Calix[8]arene Supramolecular Catalyst, *ChemCatChem*, 2022, **14**, e202200662.

[22] K. Gaalswyk and C. N. Rowley, An explicit-solvent conformation search method using open software, *PeerJ*, 2016, **4**, e2088.

[23] R. A. Talmazan and M. Podewitz, PyConSolv: A Python Package for Conformer Generation of (Metal-Containing) Systems in Explicit Solvent, *J. Chem. Inf. Model.*, 2023, **63**, 5400–5407.

[24] Y. Basdogan and J. A. Keith, A paramedic treatment for modeling explicitly solvated chemical reaction mechanisms, *Chem. Sci.*, 2018, **9**, 5341–5346.

[25] T. D. Kühne, Second generation Car–Parrinello molecular dynamics, *WIREs Comput. Mol. Sci.*, 2014, **4**, 391–406.

[26] J. R. Pliego and J. M. Riveros, Hybrid discrete-continuum solvation methods, *Wiley Interdiscip. Rev. Comput. Mol.*, 2020, **10**, 25.

[27] S. Spicher, C. Plett, P. Pracht, A. Hansen and S. Grimme, Automated Molecular Cluster Growing for Explicit Solvation by Efficient Force Field and Tight Binding Methods, *J. Chem. Theory Comput.*, 2022, **18**, 3174–3189.

[28] G. N. Simm, P. L. Turtscher and M. Reiher, Systematic microsolvation approach with a cluster-continuum scheme and conformational sampling, *J. Comput. Chem.*, 2020, **41**, 1144–1155.

[29] M. Steiner, T. Holzknecht, M. Schauperl and M. Podewitz, Quantum Chemical Microsolvation by Automated Water Placement, *Molecules*, 2021, **26**, 1793.

[30] C. N. Nguyen, T. K. Young and M. K. Gilson, Grid inhomogeneous solvation theory: Hydration structure and thermodynamics of the miniature receptor cucurbit 7 uril, *J. Chem. Phys.*, 2012, **137**, 17.

[31] X. Zhang, K. Chen, Z. Sun, G. Hu, R. Xiao, H.-M. Cheng and F. Li, Structure-related electrochemical performance of organosulfur compounds for lithium–sulfur batteries, *Energy Environ. Sci.*, 2020, **13**, 1076–1095.

[32] M. Gay, P. Carato, M. Coevoet, N. Renault, P.-E. Larchanché, A. Barczyk, S. Yous, L. Buée, N. Sergeant and P. Melnyk, New phenylaniline derivatives as modulators of amyloid protein precursor metabolism, *Bioorg. Med. Chem.*, 2018, **26**, 2151–2164.

[33] G. Chakraborti, S. Paladhi, T. Mandal and J. Dash, "On Water'' Promoted Ullmann-Type C–N Bond-Forming Reactions: Application to Carbazole Alkaloids by Selective N-Arylation of Aminophenols, *J. Org. Chem.*, 2018, **83**, 7347–7359.

[34] A. Bartoszewicz, C. D. Matier and G. C. Fu, Enantioconvergent Alkylations of Amines by Alkyl Electrophiles: Copper-Catalyzed Nucleophilic Substitutions of Racemic α-Halolactams by Indoles, *J. Am. Chem. Soc.*, 2019, **141**, 14864–14869.

[35] A. Berlanga-Vázquez, R. A. Talmazan, C. A. Reyes-Mata, E. G. Percástegui, M. Flores-Alamo, M. Podewitz and I. Castillo, Conformational Effects of Regioisomeric Substitution on the Catalytic Activity of Copper/Calix[8]arene C–S Coupling, *Eur. J. Inorg. Chem.*, 2023, **26**, e202200596.

[36] C. Bannwarth, S. Ehlert and S. Grimme, GFN2-xTB-An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions, *J. Chem. Theory Comput.*, 2019, **15**, 1652–1671.

[37] R. A. Talmazan, J. Gamper, I. Castillo, T. S. Hofer and M. Podewitz, From Data to Chemistry: Revealing Causality and Reaction Coordinates through Interpretable Machine Learning in Supramolecular Transition Metal Catalysis ChemRxiv, 2024. https://doi.org/10.26434/chemrxiv-2024-nd20j.

Prof. Dr. Maren Podewitz

Maren Podewitz completed her undergraduate studies in chemistry at the Friedrich-Schiller University Jena, Germany, where her interest in theoretical chemistry led her to join the group of Prof. Markus Reiher at the ETH Zurich for her master's thesis. After receiving her MSc in Chemistry from Jena in 2007, she continued her doctoral studies in Markus Reiher's group, focusing on structure-determining interactions in cluster chemistry, and received her PhD from ETH Zurich in 2010. In 2011, she joined the computational chemistry lab of Prof. Ken N. Houk at UCLA as a DAAD postdoctoral fellow.

In 2012, discouraged by limited job prospects in academia, Maren moved to industry as a quantitative risk analyst at a Swiss insurance company, where she developed skills in statistical modeling. Realizing her passion for research, she returned to academia in 2014 as a postdoctoral fellow at the University of Innsbruck, supported by a Lise-Meitner grant. Shifting her focus to catalysis and predictive modeling of complex systems, she established her independent research group in Innsbruck before accepting an assistant professor position at TU Wien in 2021. Her group now focuses on the development of operando models for homogeneous catalysis. Her research has been awarded with the Chemistry Europe Fellow distinction and the ACS COMP OpenEye Cadence Molecular Sciences Outstanding Junior Faculty Award in 2024.

What inspired you to pursue an academic career and when did you know that is what you wanted to do?
I was drawn to science from an early age and knew in my early teens that I wanted to study chemistry. As a graduate student and during my first postdoctoral fellowship, I enjoyed research, but I doubted that I had what it took to succeed in academia, especially given the slim chances of securing a tenure-track position. These concerns led me to leave academia after my first postdoc. During my time at the insurance company, however, I realized not only how much I missed working on challenging problems in an international scientific environment, but also that I couldn't let my fear of failure stop me from pursuing my dream of an academic career. So I decided to give it another try and returned to academia.

How did you come up with your research topic?
With a background in quantum chemistry and extensive postdoctoral experience in biomolecular simulations, it was a logical progression to combine methodologies from both fields to tackle a new topic. I was particularly interested in transition-metal catalysis because of its critical role in the development of sustainable chemical processes. Starting with a small team, I designed a research project that was both well-defined and flexible enough to allow the exploration and development of novel computational approaches.

Why did you decide for this particular funding body and what was the application process like?
My somewhat unconventional career path and focus on basic science limited my funding options. I found that a Principal Investigator project from the Austrian Science Fund (FWF) was the ideal choice. This funding not only allowed me to establish myself as an independent PI, but also gave me the flexibility to move the project from Innsbruck to Vienna after securing my tenure-track position there.

What advice would you give to someone wanting to stay in academia at the beginning of their PhD?
Pursue your doctoral studies and make the most of this time to gain knowledge and skills. Look for research opportunities to see if you enjoy the process. Consider a postdoctoral position that will allow you to explore a new area and to gain additional expertise. Aim to secure independent funding as early as possible to establish your research career.

BUNSEN-MAGAZIN · 27. JAHRGANG · 1/2025

Julia Westermayr

Advancing the Frontiers of Photochemistry Through Machine Learning

Light is one of the most abundant sources of energy on Earth and therefore, a driving force behind a variety of fundamental processes. Its influence ranges from energy harnessing in photosynthetic organisms to applications in solar cell technology. Consequently, photochemical reactions are crucial not only for the maintenance of ecosystems but also for the advancement of modern technologies. This interface between nature and technology puts photochemistry at the center of efforts to tackle some of the most pressing global challenges of our time, such as combating climate change and addressing the ongoing energy crisis [2, 3].

Despite the enormous potential of photochemistry, a complete understanding of many light-induced processes is still difficult to achieve and requires both experimental and theoretical efforts. Figure 1 illustrates the variety of processes that can occur following light excitation. As can be seen, upon light absorption, an electron is excited to a higher electronic state with the same spin multiplicity (singlet states are shown in blue in Figure 1). Ultrafast transitions, such as internal conversion between electronic states of the same spin multiplicity or intersystem crossing between states of different spin multiplicity (triplet states are shown in reddish color), can prevent photodamage, while other processes that occur on longer time scales, such as fluorescence and phosphorescence, can lead to photodamage. Thus, understanding the types of transitions that take place after light excitation can help us understand why molecules are photostable or not, and consequently why some motifs are conserved in biological systems in nature, potentially providing information for the development of artificial counterparts, for example for energy harvesting [1, 4, 5].

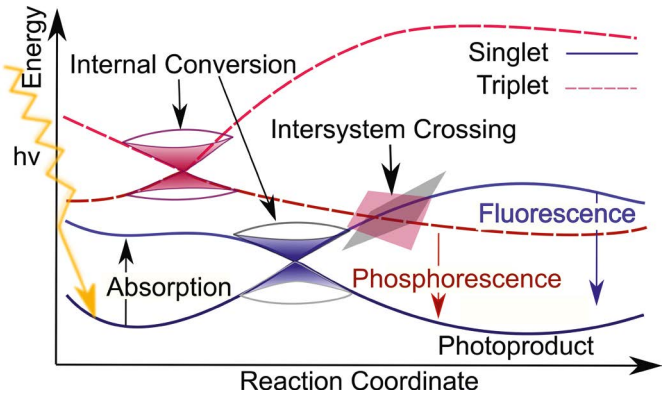


Fig. 1: Photochemical processes that can take place after light excitation. Reddisch dashed lines show triplet states and blue lines illustrate singlet states. Nonradiative transitions between states of same spin multiplicity are called internal conversion and between singlet and triplet states refer to intersystem crossing. Copyright: taken from Ref. 1 under CC-BY.

To probe photochemical reactions, experimental techniques, such as pump-probe or UV/vis absorption spectroscopy, are powerful tools by providing insights into how molecules interact with light. The spectra obtained from these experiments often represent ensemble averages and are thus complex to interpret, often requiring expert knowledge. This is where theoretical simulations can significantly improve our understanding. However, theoretical simulations come with a number of challenges. First of all, realistic molecular systems are large and inherently complex, making it extremely difficult to accurately model their light-induced reactions. Thus, larger systems, like proteins or DNA, need to be broken down into simpler components, such as individual chromophores, amino acids or DNA bases, respectively, which serve as more manageable models for theoretical investigations. This approach allows researchers to combine experimental observations with theoretical insights. However, even the simulation of these simplified models are resource-intensive as molecular dynamics relies rely on quantum chemical calculations at each time step (see Figure 2). Even with mixed quantum-classical nonadiabatic molecular dynamics methods like the surface hopping approach by Tully [6, 7], where atoms move classically on potential energy surfaces computed with quantum chemistry, the computational cost is so high that it limits studies to timescales of a few hundred femtoseconds and molecular structures with only a few dozen atoms. For

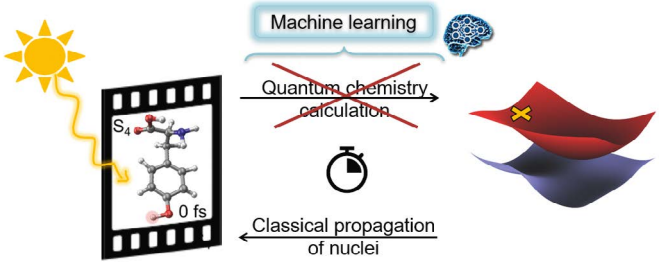


Fig. 2: Typical mixed quantum-classical photodynamics simulation, where the calculation of potential energy surfaces by quantum chemistry is replaced with machine learning. Copyright: Julia Westermayr.

Juniorprof. Dr. Julia Westermayr
Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie der Universität Leipzig
Theoretische Chemie des Materialdesigns
Philipp-Rosenthal-Straße 31, Raum E-047
Linnestr. 2, 04103 Leipzig
julia.westermayr@uni-leipzig.de

Zurück zum Inhaltsverzeichnis

example, simulating the dynamics of a single amino acid such as tyrosine when excited by light for just 10 picoseconds - equivalent to a trillionth of a second - using quantum chemical multi-reference methods on a supercomputer would take around 10 years [8]. This limitation hampers our ability to fully explore and understand the detailed mechanisms behind photochemical reactions, especially in larger and biologically relevant systems. Addressing these computational bottlenecks requires new approaches that are able to cope with the complexity and scale of photochemical processes.

Machine learning photochemistry

Machine learning (ML) offers a transformative solution by learning the relations between molecular structures and potential energy surfaces, enabling the replacement of quantum chemical calculations in molecular dynamics simulations (Figure 2). One part of our work is to develop such ML models that predict photochemical properties based on molecular structures of organic chromophores [9-13], allowing us to efficiently simulate systems such as the methylenimmonium cation, a model for cis-trans isomerization that is critical for human vision [13]. In addition, our work on the photodynamics of the amino acid tyrosine has uncovered “roaming atoms” - highly reactive radicals that can move around a molecule and trigger potentially harmful reactions [8].

However, while ML has proven effective in assisting the study of photodynamics for small organic molecules, extending these methods to larger, more complex systems remains elusive. Some of the main hurdles stem from both the inherent complexities of photochemical reactions and limitations in existing computational approaches that also hamper comprehensive data collection. One key challenge is for instance the modeling of conical intersections (see Figure 3), which are regions where two potential energy surfaces become degenerate. These regions are critical for electronic transitions, but non-smooth, leading to a break down of the underlying Born-Oppenheimer approximation. This makes it not only difficult to obtain accurate data in these regions for ML model training, but also difficult to model with ML [1]. In addition, the couplings between two potentials, i.e., nonadiabatic couplings, that are crucial for accurately capturing transitions between states, are inverse proportional to the energy gap, hence approach infinity at a conical intersection [12]. In order to improve the modeling of these regions, the group is developing ML algorithms, in collaboration with Prof. Dr. Christoph Ortner from the University of British Columbia, that can better model these cusps [14]. One way is for instance by multiplying with the associated energy gap that smoothens couplings (dashed blue line in Figure 3) or via internal ML-based Hamiltonian matrices that can form the original potential energy surfaces via mathematical transformations [14], e.g., diagonalization [9].

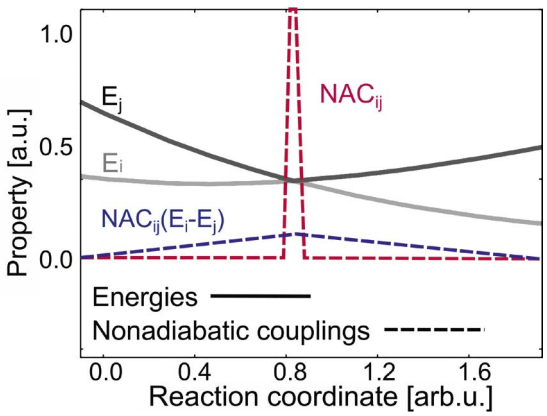


Fig. 3: A conical intersection where two energy states, Ei and Ej, approach each other and become degenerate. Couplings (reddish dashed lines) approach infinity at these regions and can be smoothened by multiplication with the energy gap. Image taken from ref. 12 under CC-BY.

Better generalization for excited-state ML: Towards larger systems and longer time scales

Another major obstacles is the lack of sufficient reference data, especially of larger systems like peptides or proteins, which is, however, essential for training accurate ML models. While ML models for ground-state simulations exist that can learn from small building blocks and predict properties of larger ones [15, 16], the same has not yet been achieved for excited states. Thus, the group focuses on the development of ML for better generalization and transferability within excited-state potentials. One way to achieve better generalization is via equivariant representations, which is enabled with the MACE model [14, 17] or SPaiNN [18] (based on the equivariant deep neural network PaiNN [19]). In addition, we are also approaching this problem from another perspective. In contrast to tackling transferability in property space, we aim to develop reinforcement learning (RL) to enable transferability in geometry space [20]. Unlike traditional ML methods that rely on pre-existing datasets, RL models learn by interacting with their environment, guided by a reward system. In our case, RL models are used to replace the integrator in molecular dynamics or traditional theoretical simulations and thus drive reactions. In our preliminary work, we demonstrated that RL could predict transition states of organic reactions [20]. By training RL models on data from quantum chemistry and existing ML models or even experimental data, we hope to develop a method that generalizes across various molecular systems. Finally, to enable the simulation of larger systems, we approach the problem from a third viewpoint and develop mixed quantum mechanics/molecular mechanics methods (QM/MM), where the quantum mechanics part is replaced by ML, enabling simulations of larger systems with traditional ML models for excited states [21].

These studies show, even though ML for excited states may still be in its infancy compared to ML for ground-state simulations, that the integration of ML into the study of photochemistry can open up new possibilities for the understanding and control of light-induced processes. It holds great promise for extending the time and length scales of photochemical simulations. We expect that these methods can lead to the development of new materials optimized for light harvesting, more efficient photocatalysts and will provide deeper insights into molecular behavior when exposed to light.

References

[1] J. Westermayr, P. Marquetand. Machine learning for electronically excited states of molecules *Chem. Rev.* 2021, **121**, 9873-9926. 10.1021/acs.chemrev.0c00749.

[2] V. Balzani, P. Ceroni, A. Juris. Photochemistry and Photophysics: Concepts, Research, Applications, (John Wiley & Sons, 2014). https://www.wiley.com/en-us/Photochemistry+and+Photophysics:+Concepts,+Research,+Applications-p-9783527334797.

[3] G. Kumari, X. Zhang, D. Devasia, J. Heo, P. K. Jain. Watching Visible Light-Driven CO2 Reduction on a Plasmonic Nanoparticle Catalyst *ACS Nano* 2018, **12**, 8330-8340. 10.1021/acsnano.8b03617.

[4] S. Mai, L. González. Molecular photochemistry: Recent developments in theory *Ang. Chem. Int. Ed.* 2020, **59**, 16832-16846. https://doi.org/10.1002/anie.201916381.

[5] M. Persico, G. Granucci. Photochemistry: A modern theoretical perspective, (Springer, 2018). 10.1007/978-3-319-89972-5.

[6] J. C. Tully. Mixed quantum–classical dynamics *Farad. Disc.* 1998, **110**, 407-419. 10.1039/A801824C.

[7] J. C. Tully. Molecular dynamics with electronic transitions *J. Chem. Phys.* 1990, **93**, 1061-1071. 10.1063/1.459170.

[8] J. Westermayr, M. Gastegger, D. Vörös, L. Panzenboeck, F. Joerg, L. González, P. Marquetand. Deep learning study of tyrosine reveals that roaming can lead to photodamage *Nat. Chem.* 2022, **1-6**. 10.1038/s41557-022-00950-z.

[9] J. Westermayr, R. J. Maurer. Physically inspired deep learning of molecular excitations and photoemission spectra *Chem. Sci.* 2021, **12**, 10755-10764. 10.1039/D1SC01542G.

[10] J. Westermayr, M. Gastegger, P. Marquetand. Combining SchNet and SHARC: The SchNarc machine learning approach for excited-state dynamics *J. Phys. Chem. Lett.* 2020, **11**, 3828-3834. 10.1021/acs.jpclett.0c00527.

[11] J. Westermayr, P. Marquetand. Deep learning for UV absorption spectra with SchNarc: First steps toward transferability in chemical compound space *J. Chem. Phys.* 2020, **153**, 154112. 10.1063/5.0021915.

[12] J. Westermayr, F. A. Faber, A. S. Christensen, O. A. Von Lilienfeld, P. Marquetand. Neural networks and kernel ridge regression for excited states dynamics of $CH_2NH_2^+$: From single-state to multi-state representations and multi-property machine learning models *Mach. Learn.: Sci. Technol.* 2020, **1**, 025009. 10.1088/2632-2153/ab88d0.

[13] J. Westermayr, M. Gastegger, M. F. S. J. Menger, S. Mai, L. González, P. Marquetand. Machine learning enables long time scale molecular photodynamics simulations *Chem. Sci.* 2019, **10**, 8100-8107. 10.1039/C9SC01742A.

[14] T. S. Gutleb, R. Barrett, J. Westermayr, C. Ortner. Parameterizing Intersecting Surfaces via Invariants *arXiv:1703.03864* 2024.

[15] D. P. Kovács, J. H. Moore, N. J. Browning, I. Batatia, J. T. Horton, V. Kapil, I.-B. Magdău, D. J. Cole, G. Csányi. Mace-off23: Transferable machine learning force fields for organic molecules *arXiv:2312.15211* 2023.

[16] O. T. Unke *et al.* Accurate machine learned quantum-mechanical force fields for biomolecular simulations *arXiv* 2022, *2310.03511*. https://arxiv.org/abs/2205.08306.

[17] I. Batatia, D. P. Kovacs, G. Simm, C. Ortner, G. Csányi. MACE: Higher order equivariant message passing neural networks for fast and accurate force fields *Advances in Neural Information Processing Systems* 2022, **35**, 11423-11436.

[18] S. Mausenberger, C. Müller, A. Tkatchenko, P. Marquetand, L. González, J. Westermayr. SpaiNN: equivariant message passing for excited-state nonadiabatic molecular dynamics *Chem. Sci.* 2024, **15**, 15880-15890. 10.1039/D4SC04164J.

[19] T. S. Kristof, T. U. Oliver, M. Gastegger. Equivariant message passing for the prediction of tensorial properties and molecular spectra *Proceedings of the 38th International Conference on Machine Learning* 2021, **139**, 9377-9388. https://www.semanticscholar.org/paper/00f39c314542902cd1b03842069e5d3ed441a5c3.

[20] R. Barrett, J. Westermayr. Reinforcement Learning for Traversing Chemical Structure Space: Optimizing Transition States and Minimum Energy Paths of Molecules *J. Phys. Chem. Lett.* 2024, **15**, 349-356. 10.1021/acs.jpclett.3c02771.

[21] B. Lier, P. Poliak, P. Marquetand, J. Westermayr, C. Oostenbrink. BuRNN: Buffer Region Neural Network Approach for Polarizable-Embedding Neural Network/Molecular Mechanics Simulations *J. Phys. Chem. Lett.* 2022, **13**, 3812-3818. 10.1021/acs.jpclett.2c00654.

1. What inspired you to pursue an academic career and when did you know that is what you wanted to do?

My path to an academic career was not something I had planned from the beginning. When I first started studying chemistry, I knew I wanted to pursue a PhD, but I didn't initially see myself staying in academia long-term. After my PhD, I chose to do a postdoc—not necessarily as a career strategy, but more to experience living abroad and to broaden my horizons. I believe one of my greatest advantages was remaining open to new opportunities, rather than following a narrow, predetermined path.
The turning point for me came during my PhD, specifically during an internship in Prof. Klaus-Robert Müller's research group, where I explored the intersection of artificial intelligence and chemistry. It was here that I realized the transformative potential of using machine learning to push the boundaries of photochemical simulations. However, research is not confined to academia. In fact, some of the most innovative work in AI often happens in industry. What ultimately convinced me to pursue an academic career was the profound fulfillment I found in teaching and mentoring students. The gratitude I received from students, the opportunity to guide them, and being able to play a small part in shaping their futures became incredibly rewarding. That sense of connection and impact is something I genuinely cherish and do not want to miss.

2. How did you come up with your research topic?

My research topic emerged from my curiosity about leveraging machine learning to address the computational challenges in photochemistry. During my PhD, I realized that traditional methods struggled to accurately simulate the excited-state dynamics of molecules on longer timescales. This motivated me to explore how AI could enhance our understanding of photochemical reactions and in general, chemistry. Thus, I started to investigate different machine learning algorithms rather those

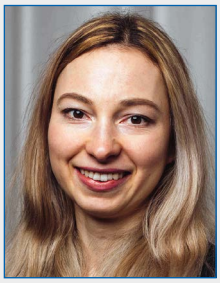
that were traditionally used and started collaborating with researchers from computational sciences and Maths.

3. Why did you decide for this particular funding body, and what was the application process like?

My funding is from the BMBF (Bundesministerium für Bildung und Forschung) and I did not apply for it, rather, the University had to apply for it and I had to apply for the open W1 tenure track position. The reason I wanted to move to Germany and applied for this tenure track position was because Germany offers a unique environment with excellent infrastructure and collaborative opportunities, making it ideal for the kind of interdisciplinary work I am passionate about.

4. What advice would you give to someone wanting to stay in academia at the beginning of their PhD?

My biggest advice would be to stay curious, resilient, and proactive. Start exploring long-term career options early on, and don't hesitate to apply for positions as they come up. Focus on building a strong foundation in your research field, but don't work in isolation—networking is key. Seek out opportunities to collaborate, attend conferences, and connect with peers and mentors. These interactions can open doors, provide fresh perspectives, and help you navigate the often challenging landscape of academia.



Juniorprof. Dr. Julia Westermayr

Julia Westermayr holds a junior professorship at Leipzig University since October 2022 and works at the intersect between artificial intelligence and (theoretical) chemistry. She is an associate member of the Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI) Dresden/Leipzig, one of the five national competence centers for AI and data science. Her doctorate was conducted in chemistry at the University of Vienna in 2020 under the supervision of Prof. Dr. Dr.h.c. Leticia González, followed by a two-year postdoctoral stay at the University of Warwick under the supervision of Prof. Dr. Reinhard Maurer, for which she received the Erwin-Schrödinger fellowship of the Austrian Science Fund (FWF). For her PhD, she received a uni:docs fellowship and was awarded the Sigrid-Peyerimhoff prize. In addition, she was awarded a scholarship from the German Scholar Organization (GSO*) for the annual Leadership Academy and is a member of the Young Forum of the Royal Saxon Society for the Sciences since this year.

BUNSEN-MAGAZIN · 27. JAHRGANG · 1/2025

Stefan Gugler

Physical-Chemistry-Inspired AI for Catalyst Design

Chemistry plays a double-edged role in the climate change battle: It is both a facilitator of the problem and a contributor to a solution. The very science that drove global industrial advancements, leading to increased carbon emissions, also holds the keys to innovations such as CO_2 capture and storage, CO_2 reduction catalysts, photovoltaics and batteries, sustainable plastics or water splitting and the hydrogen economy. Computational chemistry has—fueled by the recent incredible progress of artificial intelligence (AI)—been particularly relevant to these innovations. By simulating chemical processes, we can explore vast molecular landscapes and reactions without the need for comparably slow real-life lab experiments that often involve hazardous substances. The scalability, automatability, and efficiency of the AI-enhanced methods are almost unprecedented.

One promising approach to combating climate change is the development of efficient catalysts for water splitting, a process that generates hydrogen, a clean and renewable energy carrier:

$$2\,H_2O \rightarrow 2\,H_2 + O_2$$

Artificial photosynthesis aims to imitate the natural process by which plants convert sunlight, water, and carbon dioxide into energy-rich molecules. However, replicating this complex mechanism is a huge challenge due to the intricate electronic and structural properties of the catalysts involved, often transition metals.

Machine learning in catalyst design

The very same intricacy that makes transition metals hard to compute makes them great catalyst candidates [1]. Even the best and most accurate methods may struggle with accurately describing the complex electron structure of a transition metal complex. On top of that, these methods are very slow. But even when we sacrifice accuracy for speed and use more efficient methods like density functional theory, they are often not fast enough. One straightforward way how AI can help is by ‚simply' accelerating traditional methods from computational chemistry, e.g. by reparametrizing functionals [2], creating neural functionals [3], or running software on GPUs instead of CPUs [4]. Beyond that, many distinct novel methods have been developed without much (obvious) relation to pre-existing methods, such as graph neural networks [5] or advanced kernel methods [6]. All of these methods are general-purpose enough that they accelerate chemical research across the board, not just in the area of catalysis or climate-related research. We will now focus on one of these advanced machine learning methods that aim to *generate* rather than predict, a method which was inspired by physical chemistry: denoising diffusion models.

Dr. Stefan Gugler
Machine Learning Group & BIFOLD
Technische Universität Berlin
Marchstr. 23, D-10587 Berlin
stefan.gugler@tu-berlin.de
sgugler.ch

Denoising diffusion in molecular design

Generative models in image processing are currently to be seen all over the internet and occasionally as table of contents figures. *OpenAI*'s "Dall-E" or *Stability AI*'s "Stable Diffusion" are often the origin of those images. The user provides an input such as "an astronaut on a horse" and seconds later, an image is generated. Of course, this technology also spilled over into computational chemistry, a match made in heaven, as it turns out. Instead of predicting the properties of a molecule at hand (as described in the previous section), we do the inverse and provide an input like "a ruthenium catalyst with a high turnover number" and seconds later –hopefully– the model will produce the desired molecule.

The exciting technology behind these generative models is called denoising diffusion probabilistic models (DDPM)] [7, 8]. As the name suggests, the input image is diffused, *i.e.* noise is injected, for instance by flipping more and more pixels, one by one, until what remains is pure noise, like static on a TV. Subsequently, the model tries to reverse the noise. This also works for molecules, but instead of flipping pixels, atoms are being wiggled around. To the physical chemist, it does not come as a surprise that this was inspired [7] by Jarzynski in 1997 [9] for Helmholtz free energy estimation by transferring one distribution into another via a Markov process. Hence, DDPMs work by learning a mapping between the probability distribution of images or molecular structures and a noise distribution. This approach is very general and has been used successfully in designing molecules [10], drugs [11], or transition metal complexes [12], or finding conformers [13] or minima [14].

On a technical level, it works as follows (Fig. 1, left): The model takes the coordinates and nuclear charges of a molecule and adds random noise. The noise level is tiny (first step). We then task a neural network to learn to denoise and recover the original molecule from the slightly distorted version. This should

Zurück zum Inhaltsverzeichnis

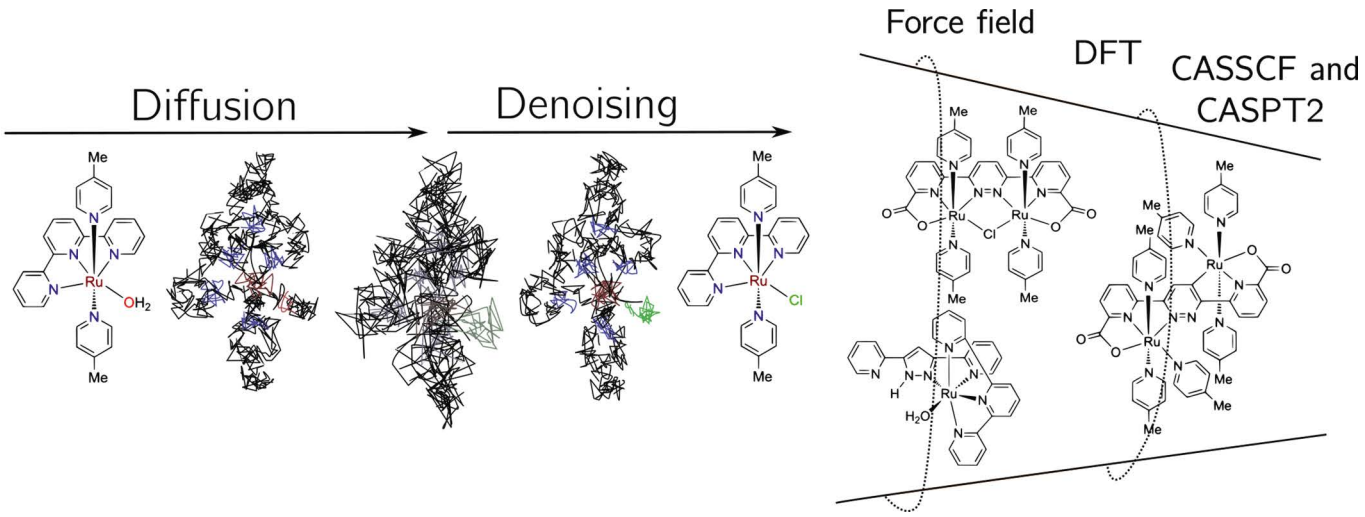


Fig. 1: Left: Diagram of one path in a denoising diffusion probabilistic model applied to a transition metal complex for water splitting. Both nuclear charges and positions are diffused, *i.e.* noise is injected. Note the water ligand in the equatorial position on the right that is diffused to a chloride ligand. Right: After generating many catalyst candidates with the diffusion model, they can be tested and evaluated with a multi-level scheme and more advanced methods. © Stefan Gugler.

be simple enough since the noise level is small. We then distort again and again, each time learning to recover the less from the noisier version. At some point, all that is left is noise (middle) and all the signal has been destroyed. If we do this for a whole data set, we obtain a new network for each step that is able to denoise its assigned step. We can now chain all these networks in a row and use them to denoise a noisy structure into a molecule (Denoising arrow). What happened on a theoretical level is that the chain of models learned a mapping between the distribution of structures in the training set and a noise distribution, usually a Gaussian. Sampling from a Gaussian is much easier than sampling from a molecular distribution. So, if we choose a starting point that is complete noise, it will denoise it and generate valid *new* molecules. This can be constrained and guided in many ways to bias the denoiser towards structures with desired properties [15], for instance to a certain potential energy surface. The obtained structures can be analyzed and pruned with standard multi-level methods (Fig. 1, right), down to computationally demanding first principles models to verify the properties of a designed candidate catalyst.

Challenges and future directions

While the advancements are promising, several challenges remain. On the technical side, it is important to note that ML models learn a distribution encoded by the empirical data. It is generally not possible to generalize arbitrarily well outside of the distribution. Multi-level approaches (Fig. 1, right) and pre-training deep learning models [16] are possible remedies. But the accurate modeling of the intricate molecular electronic structure still requires accurate quantum chemical calculations, which are computationally intensive. Last but not least, ML models often merely fit the physical observations, while traditional approaches try to model the underlying physical laws. Employing physic-based representations in ML [17] or disentangling deep neural networks with explainable AI [18] are approaches to combine strengths from both fields.

As Schilter *et al.* [19] pointed out, there are some more qualitative limitations. Both traditional computational chemistry and ML in chemistry consume a lot of energy in their simulation with diminishing returns. Korolev and Mitrofanov showed that a 28% decrease in mean absolute error for training an ML model corresponds to a 15,000% increase in the carbon footprint [20] with data centers partly to blame [21]. Even though running a calculation on a GPU accelerates it, this can lead to a higher carbon emission due to inefficient compute allocation [22]. If the result of a particular simulation cannot be employed for a real-life application, it is one step forward, two steps back in terms of emissions.

This phenomenon relates to the Jevons paradox [23], which says that improvements in efficiency can lead to an overall increase in energy consumption. In the context of computational chemistry, making ML models more efficient reduces the computational cost per simulation, effectively making it cheaper to discover new catalysts. However, this cost reduction often leads scientists to perform many more simulations than before, thereby increasing the total energy consumption despite the efficiency gains.

Conclusion

The fusion of computational chemistry and ML holds great promise for addressing climate change challenges by assisting in the discovery of efficient catalysts for processes like water splitting. These advancements enable the generation of novel molecular structures with desired properties, potentially revolutionizing renewable energy production and other sustainable technologies. Due to its computational nature, insights from theoretical and physical chemistry are particularly crucial and (re-)emerge in many statistical applications like diffusion models. Moving forward, it is important to refine these technologies further – perhaps by integrating more physics-based concepts – to ensure that our efforts to combat climate change are both expedient and environmentally responsible.

References

[1] Markus Reiher: A Theoretical Challenge: Transition-Metal Compounds, *Chimia* 2009 **63**, 3, 140.

[2] Jess Wellendorff, Keld T. Lundgaard, Andreas Møgelhøj, Vivien Petzold, David D. Landis, Jens K. Nørskov, Thomas Bligaard, Karsten W. Jacobsen: Density functionals for surface science: Exchange-correlation model development with Bayesian error estimation, *Physical Review B* 2012 **85**, 235149.

[3] James Kirkpatrick, Brendan McMorrow, David H. P. Turban, Alexander L. Gaunt, Alexandre G. D. G. Matthews, Oliver T. Unke, Eszter Ignácz, Benedek Bozsonyi, José Guaita Ruiz, Luigi Marti Ferrando, Reinhard Maurer, Félix Benveniste, Simon Neubauer, Marcel Gastegger, and Baking Soda & Ross F. Grote, Akira Ishikawa, Aron J. Cohen: Pushing the frontiers of density functionals by solving the fractional electron problem, *Science* 2021 **374**, 6573, 1385.

[4] Stefan Seritan, Christoph Bannwarth, Bryan S. Fales, Edward G. Hohenstein, Christine M. Isborn, Sara I. L. Kokkila-Schumacher, Xin Li, Fang Liu, Nathan Luehr, Nilukai Thapa, James W. Snyder Jr., Bora Ungar, Martin Head-Gordon: TeraChem: A graphical processing unit-accelerated electronic structure package for large-scale ab initio molecular dynamics, *Wiley Interdisciplinary Reviews: Computational Molecular Science* 2020 **11**, e1494.

[5] Jascha Sohl-Dickstein, Eric A. Weiss, Niru Maheswaranathan, Surya Ganguli: Deep Unsupervised Learning using Nonequilibrium Thermodynamics, arXiv:1506.02441.

[6] Jonathan Ho, Ajay Jain, Pieter Abbeel: Denoising Diffusion Probabilistic Models, arXiv:2006.11239.

[7] Oliver Schilter, Philippe Schwaller, Teodoro Laino: Balancing computational chemistry's potential with its environmental impact, *Green Chemistry* 2024 **26**, 8669.

[8] Thomas Schnake, Farnoush Rezaei Jafari, Jonas Lederer, Ping Xiong, Shinichi Nakajima, Stefan Gugler, Grégoire Montavon, Klaus-Robert Müller: Towards Symbolic XAI – Explanation Through Human Understandable Logical Relationships Between Features, arXiv preprint.

[9] Christopher Jarzynski: Equilibrium free-energy differences from nonequilibrium measurements: A master-equation approach, *Physical Review E* 1997 **56**, 5, 5018.

[10] Stefan Gugler, Markus Reiher: Quantum Chemical Roots of Machine-Learning Molecular Similarity Descriptors, *Journal of Chemical Theory and Computation* 2022 **18**, 11, 6670.

[11] Zhonglin Cao, Simone Sciabola, Ye Wang: Large-Scale Pretraining Improves Sample Efficiency of Active Learning-Based Virtual Screening, *Journal of Chemical Information and Modeling* 2024 **64**, 6, 1882.

[12] Tomer Weiss, Eduardo Mayo Yanes, Sabyasachi Chakraborty, Luca Cosmo, Alex M. Bronstein, Renana Gershoni-Poranne: Guided diffusion for inverse molecular design, *Nature Computational Science* 2023 **3**, 873.

[13] Khaled Kahouli, Stefaan Simon, Pierre Hessmann, Klaus-Robert Müller, Shinichi Nakajima, Stefan Gugler, Niklas Wolf, Andreas Gebauer: Molecular relaxation by reverse diffusion with time step prediction, *Machine Learning: Science and Technology* 2024 **5**, 3, 035038.

[14] Amira Alakhdar, Barnabas Poczos, Newell Washburn: Diffusion Models in De Novo Drug Design, *Journal of Chemical Information and Modeling* 2024 **64**, 19, 7238.

[15] Hongni Jin, Kenneth M. Merz Jr.: LigandDiff: de Novo Ligand Design for 3D Transition Metal Complexes with Diffusion Models, *Journal of Chemical Theory and Computation* 2024 **20**, 10, 4377.

[16] Minkai Xu, Lantao Yu, Yang Song, Chence Shi, Stefano Ermon, Jian Tang: GeoDiff: A geometric diffusion model for molecular conformation generation, *International Conference on Learning Representations* 2022.

[17] Emiel Hoogeboom, Victor G. Satorras, Clément Vignac, Max Welling: Equivariant diffusion for molecule generation in 3D, *Proceedings of the 39th International Conference on Machine Learning* 2022.

[18] Beth Whitehead, Deborah Andrews, Amip Shah, Graeme Maidment: Assessing the environmental impact of data centres part 1: Background, energy use and metrics, *Building and Environment* 2014 **82**, 151.

[19] William Stanley Jevons: The Coal Question: An Inquiry Concerning The Progress Of The Nation, And The Probable Exhaustion Of Our Coal Mines, 1865.

[20] Vadim Korolev, Artem Mitrofanov: The carbon footprint of predicting CO2 storage capacity in metal-organic frameworks within neural networks, *iScience* 2024 **27**, 5, 109644.

[21] Jason Grealey, Loïc Lannelongue, Woei-Yuh Saw, Jonathan Marten, Guillaume Méric, Sergio Ruiz-Carmona, Michael Inouye: The Carbon Footprint of Bioinformatics, *Molecular Biology and Evolution* 2022 **39**, 3, msac034.

Dr. Stefan Gugler

Dr. Stefan Gugler is a postdoctoral researcher at Technische Universität Berlin and BIFOLD, collaborating with Prof. Dr. Klaus-Robert Müller. His research is centered on novel machine learning methods such as probabilistic diffusion models, with an interest in explainable AI (XAI) and its applications in theoretical chemistry. In his Ph.D. research at ETH Zürich under Prof. Markus Reiher, he developed machine learning methodologies that integrated Gaussian process regression and Bayesian sampling to refine dispersion interactions between organic compounds. His work also explored the interplay between machine learning descriptors and their physical chemistry counterparts, aiming to enhance quantum chemistry predictions. Prior to his doctoral studies, he completed his Master's research at the Massachusetts Institute of Technology with Prof. Heather J. Kulik, focusing on transition metal complexes for multi-fidelity machine learning.

Carina Allacher, Siyu Fan, Marius Gerlach, Justus Metternich

Finalists of the Agnes-Pockels-PhD Award 2025

The Agnes-Pockels-PhD award recognises an outstanding PhD in Physical Chemistry and 2025 is the 6th time it will be awarded by the German Bunsen Society. The jury has the selected the four finalists – Carina Allacher from Universität Regensburg, Siyu Fan from University of Groningen, Marius Gerlach who completed his PhD at Julius-Maximilians-Universität Würzburg, and Justus Metternich who did his PhD at Ruhr-University Bochum and Fraunhofer IMS. All four finalists will present their work in the Agnes-Pockels session at the Bunsen-Tagung 2025 in Leipzig, where the award winner will be chosen. We are excited to introduce the four finalists and their research.

The yPC Editorial Team

Deciphering Multistep Photoreactions Involving Radicals and Geminate Ion Pairs

Chemical reactions are generally determined by a multitude of interactions and conditions. In order to identify new light-induced reaction pathways and make them exploitable in applications, it is indispensable to elucidate the underlying reaction steps in as much detail as possible. In this endeavor, it is often difficult to uncover the ultrafast processes after excitation together with slower reaction steps, such as bimolecular interactions. This is where mechanistic investigations on multiple time scales may prove to be beneficial. In my thesis, such an approach using time-resolved spectroscopy methods was pursued, with an emphasis on elucidating reaction mechanisms and reactivities of organoselenium molecules. For organic diselenides, it was demonstrated that upon excitation, these compounds initially undergo homolysis, as expected for such a highly symmetric molecule. However, during the time the fragments still possess significant excess energy, an electron transfer between the two structural identical fragments can occur, leading to a net heterolysis of this otherwise nonpolar bond. This reaction principle, which relies on two distinct stimuli—where the first generates a radical and the second initiates an electron transfer—has been termed *stimulated doublet electron transfer* (SDET). This concept can also be extended to carbon-selenium bonds.

A completely different reaction mechanism is involved when selenohydrins undergo a semi-pinacol rearrangement upon excitation. Here, the phenylselenyl leaving group is activated intramolecularly through a hydrogen bond between the hydroxyl group and the selenium atom. Fluorinated alcohols like hexafluoroisopropanol as solvents were found to be essential because of a pronounced enhancement of hydrogen bonding. In this way, excitation leads to splitting off of a phenylselenol radical cation instead of a neutral phenylselenyl radical, thereby enabling the rearrangement of the molecule. The studies were complemented by fruitful collaborations with colleagues in synthesis, computational chemistry, and from NMR- and EPR spectroscopy, which made it possible to gain a comprehensive understanding of the reactions.

In essence, the projects of my thesis have opened a new perspective on the understanding of the photochemistry of organoselenium compounds. New reaction pathways were identified with great appeal for applications ranging from catalysis to medicinal chemistry.

Carina Allacher

Carina Allacher studied Chemistry at the University of Regensburg and completed a research stay at the IOCB in Prague doing synthesis. She currently finishes her PhD under the supervision of Patrick Nürnberger and serves as the graduate speaker of the Collaborative Research Center 325 “Assembly-Controlled Chemical Photocatalysis”.

Institut für Physikalische und Theoretische Chemie
Universität Regensburg
Universitätsstrasse 31
93053 Regensburg
Germany

Quantum Sensing for Free Radical Generation in Living Cells and Organisms

Free radicals play a crucial role in various biological processes such as cell signalling, aging, and disease progression, but their short-lived and reactive nature makes them challenging to measure. Quantum sensing, utilizing defects in diamond, enables precise detection of magnetic signals that are translated into optical signals, offering nanoscale resolution similar to MRI imaging but at a much smaller scale.

In my thesis, I employed this state-of-the-art technology to investigate free radical generation in diverse biological contexts. These included studies on mitochondrial activity in single heart muscle cells during hypoxia and reoxygenation, free radical dynamics in human keratinocytes subjected to UVB exposure, and oxidative stress in Caenorhabditis elegans models of Huntington's disease. By using diamond-based quantum sensors, I was able to observe these processes in real-time, shedding light on the localized generation and behavior of free radicals under various conditions.

This work not only enhances our understanding of the role of free radicals in cellular and organismal physiology but also establishes quantum sensing as a versatile and precise tool for studying these elusive molecules in vivo. The insights gained from this research have broad implications, ranging from better understanding disease mechanisms to developing novel therapeutic strategies for conditions influenced by oxidative stress.

Siyu Fan

Siyu Fan is currently pursuing a PhD in Biomaterials & Biomedical Technology at the University of Groningen, working in Prof. Romana Schirhagl's research group. Prior to that, she completed her master's degree in Nanotechnology at the University of Twente.

Biomaterials and Biomedical Technology (BBT)
Building 3215, University Medical Center Groningen
Antonius Deusinglaan 1
9713 AV Groningen
The Netherlands

Spectroscopy of Fulminic Acid, HCNO, With VUV- and Soft X-ray Radiation

Fulminic acid HCNO, is an unstable molecule which rapidly decomposes at temperatures above 0 °C. Still, it has been known since the year 1800, when it was first synthesized by Edward Howard. HCNO has served generations of chemists as a model molecule to understand new concepts and techniques such as isomerism or quantum chemical calculations. In recent years, research on HCNO is motivated by astrochemistry due to its astronomical detection in 2009.

In my thesis, I used four different experimental techniques to uncover the interaction of HCNO with VUV- and soft X-ray radiation, i.e. radiation that is also present in the interstellar medium. We conducted these experiments at the synchrotron radiation facilities Swiss Light Source in Villigen, CH and SOLEIL in Saint-Aubin, FR, where we synthesized HCNO samples on-site *via* gas-phase pyrolysis.

We measured VUV photoelectron spectra up to a binding energy of 22 eV. The transition into the Renner-Teller distorted $X^+ {}^2\Pi$ ground state of $HCNO^+$ were simulated using wavepacket dynamics simulation. We could also show that dissociative photoionization of $HCNO^+$ yields the fragments HCO^+, NCO^+, NH^+ and CO^+. With the aid of quantum-chemical calculations, we were able to determine possible isomerization mechanism for the formation of HCO^+ and NCO^+.

Using soft X-ray radiation, we recorded X-ray photoelectron spectra of HCNO and investigated the subsequent Auger-Meitner effect *via* Auger electron spectroscopy. The spectra were assigned with simulations. In addition, we investigated the fragmentation following the Auger-Meitner process and could observe that ionization of the C1s electron led to more pronounced dissociation compared to ionization of either the N1s or O1s electron.

In summary, we successfully synthesized the reactive molecule HCNO and studied it with a range of different experimental setups. This research provides a comprehensive picture of the interaction of HCNO with VUV- and soft X-ray radiation. It also shows that the subsequent fragmentation may form reactive ions, which can lead to further reactions in the interstellar medium.

Dr. Marius Gerlach

Marius Gerlach studied Chemistry at the Julius-Maximilians-Universität Würzburg. There he completed his PhD in the group of Prof. Ingo Fischer. He is now working as a Walter Benjamin Fellow at the Radboud University, Nijmegen, NL.

HFML-FELIX
Toernooiveld 7
6525 ED Nijmegen
The Netherlands

Near-Infrared Fluorescent Nanosensors for Pathogen Detection

Sensors are a key technology for progress in medicine, environmental monitoring, and are particularly important for biomedical diagnostics. Moreover, they are based on fundamental physical-chemical principles that are universally applicable to many other processes. In my thesis, I investigated processes at polymer-nanomaterial interfaces and utilized the underlying mechanisms to develop new types of optical nanosensors.

The first part of my work focused on: i) the rational assembly of near-infrared (NIR) fluorescent single-walled carbon nanotube (SWCNT) sensors, and ii) the optimization of the sensor-selectivity with so-called guanine quantum defects. Typically, SWCNTs are modified through noncovalent chemistry. However, noncovalent chemistry has several limitations and prevents a consistent way to molecular recognition and reliable signal transduction. By utilizing DNA strands with capture sequences, it was possible to bind and position recognition units on SWCNTs. An interaction between analytes and the recognition unit changed the SWCNT fluorescence, and the use of a capture sequences allowed a quick adaptation (≈ 2 h) of the sensors to different analyte classes (e.g., DNA, bacterial siderophores, and proteins). To enhance the selectivity of the sensors, guanine quantum defects were introduced to covalently fixate DNA with guanine bases as anchor sequences on the nanotube. This reduced unspecific interactions and led to an increase of the sensor selectivity. Additionally, hybridization on the connected capture sequence increased with the length of the capture sequence (20 > 10 ≫ 6 bases) and provided a rational pathway for tailored assembly.

In the second part, I used the nanosensors as signal amplifiers for absorption-based detection methods. By modifying SWCNTs with specific (bio)polymers, it was possible to create sensors for the substrates/products of horseradish peroxidase (HRP) and β-galactosidase. Compared to the classical absorption-based readout, these sensors were able to amplify signal changes of enzymatic reactions. It allowed us to follow enzymatic reactions of HRP below the limit of detection of the visible spectrum in the NIR (≈ 1000 nm). An adsorption-based theoretical model fitted the observed signals and corroborates the sensor-based enhancement mechanism. Conceptually, this use of nanosensors represented i) a novel approach to signal translation into a different spectral range, and ii) offered a simultaneous nonlinear signal amplification (up to ≈ 120x). Overall, this effect, which we called SENSAT (sensor-based signal amplification and translation), improves the readout of enzymatic reactions.

Dr. Justus Metternich

Justus Metternich studied biotechnology in Darmstadt (2014–2017) and chemistry in Uppsala (2018–2020). In 2024, he received his Ph.D. in Physical Chemistry at Ruhr-University Bochum and Fraunhofer IMS (with Prof. Sebastian Kruss). His research focuses on chemical modifications of fluorescent nanomaterials, rational assembly of soft interfaces, and their use as sensors.

Ruhr-Universität Bochum
Physikalische Chemie 2
Universitätsstr. 150
44801 Bochum
Germany

Your Publications: Communicated!

Welcome to "*your Publications: Communicated!*", the new Bunsen-Magazine category in which we invite early career researchers to briefly summarize their newest research paper. Below, you can find the first two contributions we have selected. The first one is about heterometallic oxo-clusters for thin film applications in electronic devices and the second contribution details the deposition of conductive MOF nanostructures for micro supercapacitor integration.

If you are also interested in sharing your research with the Bunsen community, just send us a short one paragraph summary of your paper as well as a meaningful figure to ypc@go.bunsen.de and we will share the best ones here in the Bunsen-Magazin and across our yPC social media channels!

yPC Editorial Team

Jonas Lorenz, Maximilian Seiß

Heterometallic Oxo-Clusters for Future Thin Film Applications in Electronic Devices

Maximilian Seiß, Jonas Lorenz, Sebastian Schmitz, Marco Moors, Martin Börner and Kirill Yu. Monakhov, Synthesis and structures of cobalt-expanded zirconium- and cerium-oxo clusters as precursors for mixed-metal oxide thin films. *Dalton Trans. 2024*, **53**, 8454 – 8462, doi: https://doi.org/10.1039/D4DT00328D.

In modern electronics, memory technologies like resistive random-access memory (ReRAM) are critical for data storage and processing. A typical ReRAM cell is designed as a simple metal–insulator–metal structure in which metal oxides play a vital role as the switching material. It has been shown that doping these oxides and using multiple metal-oxide layers can significantly enhance the performance of these devices. However, the fabrication of these so-called complex metal oxide (CMO) layers often demands energy-intensive processes at elevated temperatures, posing challenges for sustainable production. In our research group, we aim to address this issue utilizing molecular single-source precursors which will be converted into intrinsically mixed CMO layers. Accordingly, our study introduces cobalt-expanded zirconium (Zr_6Co_6) and cerium (Ce_3Co_2)-oxo clusters as potential molecular precursors. These precursors enable a solution-based deposition that offers lower-energy processing while ensuring precise control over material composition. We present the synthesis of the novel mixed-metal clusters starting from simple hexanuclear zirconium- or cerium-complexes and cobalt carboxylates. The new complexes were fully characterized, and their thermal stability in bulk was explored. Furthermore, first adsorption studies on Au(111) and industrial-relevant SiO_2/Si surfaces were performed. This work indicates the potential suitability of Zr_6Co_6 as a candidate for generating new and well-defined CMOs with potential use for resistive memory applications. Future studies will involve creating well-defined CMO layers by using single-molecule precursors to examine their structural and electronic properties as a low-energy and temperature approach, which is crucial for environmentally friendlier high-end technical applications.

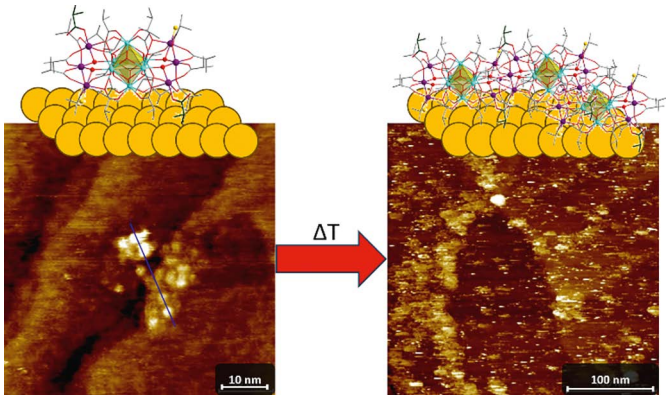


Fig. 1: Schematic representation of the deposited Zr_6Co_6 precursor with the corresponding STM image on an Au(111) surface (left) and the agglomeration that occurred on the same sample after annealing to 200 °C under UHV conditions (right).

Jonas Lorenz
Leibniz-Institut für Oberflächenmodifizierung e.V. (IOM)
Permoserstraße 15, D-04318 Leipzig
jonas.lorenz@iom-leipzig.de
https://www.iom-leipzig.de/forschung/inkubator-explorative-projekte.html

Maximilian Seiß
Georg-August-Universität Göttingen, Institut für Anorganische Chemie
Tammannstraße 4, D-37077 Göttingen
maximilian.seiss@uni-goettingen.de
https://www.uni-goettingen.de/de/startseite/611492.html

Géraldine Chanteux

A Direct Anodic Deposition of Conductive MOF Nanostructures for Micro Supercapacitor Integration

Sepideh Behboudikhiavi, Géraldine Chanteux, Binson Babu, Sébastien Faniel, Florent Marlec, Kevin Robert, Delphine Magnin, Fabio Lucaccioni, Joel Ojonugwa Omale, Petru Apostol, Luc Piraux, Christophe Lethien, and Alexandru Vlad, Direct Electrodeposition of Electrically Conducting $Ni_3(HITP)_2$ MOF Nanostructures for Micro-Supercapacitor, Small 2024, **20**, 2401509, doi: https://doi.org/10.1002/smll.202401509

Conductive metal organic frameworks (MOFs) have emerged as prominent candidates in the race for functional materials effectively tackling the challenges associated with energy storage. Among all these materials, $Ni_3(HITP)_2$ has particularly gained interest in the past years as a capacitive material, due to the exceptional combination of large surface area (>1.000 m^2/g) with very high electrical conductivities (>50 S/cm). With the realm of portable devices in full expansion in modern societies, it becomes critical to search for appropriate techniques to incorporate films as active materials in (micro-)supercapacitors. Mainly used in capacitor devices, carbon materials are hard to synthesize in films and do not meet challenges of the ever-growing miniaturization. To take advantage of the capacitive properties of $Ni_3(HITP)_2$, electrochemical deposition is considered as a premium technique for the synthesis of conformal films on any small and/or large surfaces, and in the 3D space. In this project, we developed a direct non-sacrificial anodic deposition of $Ni_3(HITP)_2$ in both aqueous and organic-based electrolytic baths. The examination of the synthesis parameters is systematically studied using a indium-tin-oxide coated working electrode, and highly crystalline MOF films are grown in a homogeneous and pure phase. The deposition is feasible on the surface of other flat substrates (Pt coated electrode, carbon cloth, stainless steel), and the growth of core-shell Pt-$Ni_3(HITP)_2$ nanowire and $Ni_3(HITP)_2$ nanotube networks is achievable with a good mechanical stability. Finally, symmetrical $Ni_3(HITP)_2$ deposition on both interdigits of a micro supercapacitor chip is performed and the device shows very good stability over 1.000 cycles, reaching reported values of capacitance per amount of deposited material.

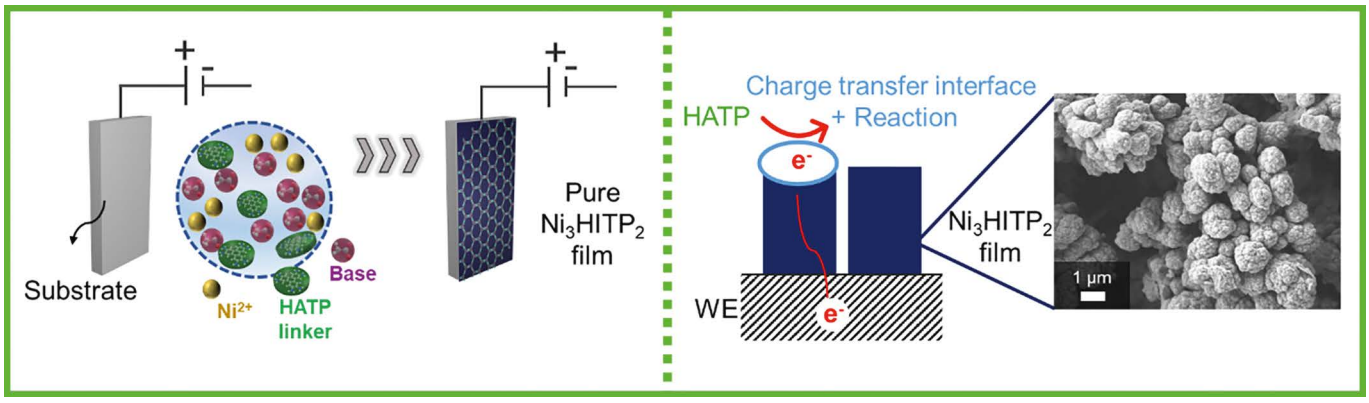


Fig. 1: Schematic illustrating (left) the anodic deposition strategy for the synthesis of conformal $Ni_3(HITP)_2$ films, and (right) zoom-in on the charge transfer interface mechanism for the crystallization growth with a characteristic SEM image of the $Ni_3(HITP)_2$ film. Adapted from © 2024 Wiley.

Mrs. Géraldine Chanteux
Institute of Condensed Matter and Nanosciences (IMCN),
Molecular Chemistry, Materials and Catalysis (MOST) Division
Université catholique de Louvain
Place Louise Pasteur, 1/L4.01.02
geraldine.chanteux@uclouvain.be

Noah Al-Shamery, Katharina Meyer, Tobias Dickbreder, Florian Schneider, yPC Team

yPC Report 2024

2024 has been another eventful year for the *young Physical Chemists* (yPC). We've embraced new formats, built on our successes, and strengthened connections within the scientific community. Let's take a look back at the highlights!

The Team

Our core team has increased to nine members since the last Bunsen-Tagung and our two speakers are currently Katharina Meyer and Noah Al-Shamery. We had one more member join very recently: Welcome to the team Ekaterina Salikhova! We always look forward to having new members joining us, so please get in contact with us via email (ypc@go.bunsen.de), social media or in person at the Bunsen-Tagung 2025 in case you are interested.

New projects: *yPC KarriereRadio*

This year marked a significant shift as we transitioned our *yPC meets Industry and Science* seminar series into the podcast format **yPC KarriereRadio**. Hosted by Carolin Müller and Christina Tonauer, this new initiative brings career advice and scientific insights directly to listeners across audio platforms like Spotify.

As part of our ongoing collaboration with *Nachrichten aus der Chemie*, we featured interviews with the contributors to this year's *Trendberichte Physikalische Chemie* in our *yPC KarriereRadio*. Prof. Tobias Beck (University of Hamburg), Dr. Daniel Keefer (MPI Mainz), and Prof. Klaus Boldt (University of Rostock) shared their cutting-edge research and personal career trajectories in engaging podcast episodes. The *Trendberichte* remain accessible in the respective issue of *Nachrichten aus der Chemie* – and we highly recommend checking out the podcast for a fresh perspective on physical chemistry!

Bunsen-Tagung 2024: Bigger and better

The Bunsen-Tagung 2024 in Aachen was very successful with an expanded yPC program that built on last year's achievements. Former yPC co-speaker Mathias Micheel opened the conference with a speech highlighting our activities. Two well-received workshops kicked off the event: Patrick Koy from MLP offered practical advice on navigating the transition from academia to industry, while Dr. Bee Hockin from *Physical Chemistry Chemical Physics* (PCCP) led a session on "*How to Publish with Impact,*" equipping attendees with strategies for maximizing the visibility of their research.

Another highlight was this year's yPC Forum, which explored job opportunities after a completed PhD. We were thrilled to welcome speakers Thomas Czirnich (RWTH Career Service), Jürgen Kolenda (Coherent), and Johannes Klütsch (FEV), who shared valuable insights into career paths in academia, industry, and beyond. Active participation from the audience made this a lively and informative discussion.

Top left: yPC members supporting the DBG booth during the Bunsen-Tagung 2024. Top right: yPC Forum at the Bunsen-Tagung in Aachen. Bottom: Group picture of the yPC at the conference dinner. (Copyright: yPC/Noah Al-Shamery)

Our involvement extended to chairing the *25th Anniversary DBG & PCCP* session, which featured presentations by Franziska Kilchert, Sabine Wenzel, Melanie Schnell, and Christoph Kerzig, celebrating a milestone for Physical Chemistry Chemical Physics. The conference concluded with the Agnes-Pockels-PhD Award session, a showcase of outstanding doctoral research. We congratulate all four participants on their excellent contributions and Karl Michael Ziems for winning the award!

During the yPC General Assembly, Noah Al-Shamery was elected as a new yPC co-speaker, taking the baton from Mathias, who completed his two-year term. Thank you, Mathias, for your dedication, and congratulations, Noah! The next yPC General Meeting in early 2025 will see the election of a new yPC co-speaker, as Katharina completes her second consecutive term.

We are currently busy planning different events for the Bunsen-Tagung 2025 in Leipzig, so stay tuned for our workshops, yPC Career session, Agnes-Pockels-PhD award, and the networking evening!

yPC strengthening international connections

This year, yPC significantly expanded its international presence, building stronger ties with organizations across Europe and beyond. The European Young Chemists' Network (EYCN), a key partner in fostering collaboration among early-career chemists, has been central to these efforts. Representing yPC, Noah Al-Shamery attended the EYCN Delegate Assembly held at the historic RSC Burlington House in London. The assembly provided a platform to exchange ideas, collaborate on initiatives, and explore strategies for promoting scientific communication and engagement across Europe. The inclusion of yPC to EYCN was highlighted in an article of the EuChemS Magazine Plus (https://www.magazine.euchems.eu/bunsen-eycn/).

yPC Delegate Noah Al-Shamery discussing with other EYCN member society delegates at the EYCN Delegate Assembly 2024 at the RSC Burlington House in the UK. (Copyright: Royal Society of Chemistry (RSC))

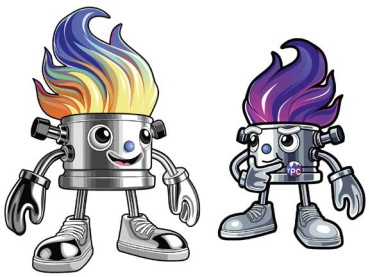
Christina's participation in the *GÖCH Chemietage 2024* (Austrian Chemistry Days) in Graz further strengthened ties with the young chemist division of the Austrian Chemical Society (GÖCH), and Noah continued building our Network with the German Young Chemistry Forum (JCF) at the Spring and Fall meetings of their society respectively. In addition to these in-person engagements, Noah also regularly represented yPC at online meetings organized by the European Institute for Industrial Leadership (EIIL). Looking ahead, yPC plans to continue building these bridges, with the goal of creating even more opportunities for members to engage with international initiatives, participate in global discussions, and enhance their scientific careers.

yPC on social media

This year, our social media presence continued to grow. With accounts on Instagram (@ypc_bunsen), Mastodon (https://physchem.science), and LinkedIn, we aim to reach early-career members across diverse platforms. These channels are vital for sharing updates on events, podcast episodes, and new initiatives like the regular "*Your Publications: Communicated!*" column in the Bunsen-Magazin.

Introducing... Burny, the new DBG/yPC mascot!

To end things off – and you may have spotted it on the cover of this magazine already – yPC was hard at work to design a gender-neutral mascot character that you will see in future publications of the DBG and yPC: Meet Burny! Inspired by the namesake of our very own society, you can expect Burny switching up their flame depending on their mood and the situation, to be featured on various DBG/yPC designs in the future!



The DBG- (left) and yPC- (right) version of our new mascot character: Burny. (Copyright: yPC/Simon Sprengel)

We need YOU at yPC!

2024 has been a busy year for us, and 2025 will be even better. Since our core team size has been growing rapidly, we have restructured into 7 different task groups to tackle the key topics relevant to yPC: Bunsen-Magazin, Events, Supporting Structure, KarriereRadio, Recruitment and Outreach, Social Media, and EYCN. If any of these task groups seem interesting to you, or if you have completely new ideas for events, excursions, seminars, or Bunsen-Magazin articles, we are happy to have you in our core team! yPC is always looking for new members.

You have expertise in event planning or graphic design, or any other comparable skill suitable to our task groups? Then why not join us and help us design and organize! You will enjoy talking to our very diverse core team members spanning from people in industry, to junior research group leaders, and graduate/postgraduate students in physical chemistry. Don't hesitate to contact us *via* e-mail (ypc@go.bunsen.de) or any of our social media, or talk to us directly at the upcoming Bunsen-Tagung in Leipzig! This has been your yPC team: Signing off!

Ludwig A. Kibler, Timo Jacob

Internationale Bunsen-Diskussionstagung „Facets of Electrodeposition“

3. Gerischer-Kolb-Symposium 2024 auf Schloss Reisensburg

Vom 16. bis zum 19. Oktober 2024 fand auf Schloss Reisensburg, (Abb. 1) dem Wissenschaftszentrum der Universität Ulm, das dritte Gerischer-Kolb-Symposium zum Thema „Facets of Electrodeposition – From Fundamentals to Applications“ statt. Insbesondere die Metallabscheidung besitzt enorme technologische Bedeutung (Galvanische Industrie) und ist gleichzeitig mit etlichen grundlegenden Fragestellungen verknüpft. Sowohl Heinz Gerischer (1919-1994) als auch Dieter M. Kolb (1942-2011) haben auf diesem Gebiet wegweisende Beiträge geleistet, denken wir an die Untersuchung von Abscheidemechanismen, die Unterpotentialabscheidung von Fremdmetallen zur Bildung von pseudomorphen Schichten oder den Einsatz des Rastertunnelmikroskops zur *in-situ* Untersuchung der Anfangsstadien der Metallabscheidung oder zur Nanostrukturierung von Oberflächen mithilfe der STM-Spitze.

Abb. 1: Die Tagungsstätte Schloss Reisensburg © Ludwig A. Kibler.

Kolb selbst hatte seit 1999 im Drei-Jahres-Rhythmus insgesamt fünf Gerischer-Symposien im Harnack-Haus in Berlin zu Ehren seines Mentors durchgeführt. Dort fand 2014 das erste Gerischer-Kolb-Symposium zum Thema *Electrochemical Surface Science* statt. Das 2. Gerischer-Kolb-Symposium rund um Bioelektrochemie wurde bereits auf Schloss Reisensburg veranstaltet. Nach den unvorhersehbaren Corona-bedingten Verschiebungen setzen die Organisatoren Timo Jacob und Ludwig Kibler die Tradition der Konferenzreihe fort, um grundlegende Fragestellungen der aktuellen Elektrochemie in einer Internationale Bunsen-Diskussionstagung zu behandeln.

Eine große Themenvielfalt von der Grundlagenforschung bis zur Anwendung wurde in einem kompakten Programm mit insgesamt acht Sitzungen und 23 Vorträgen behandelt und folgenden Bereichen zugeordnet: Elektrodeposition, Batterien, (Elektro-) Katalyse, Grenzflächen, Methoden. Längst etablierte Modelle wurden neu beleuchtet und neue Sichtweisen vorgestellt. Im Wesentlichen wurde immer wieder deutlich, dass eine detaillierte Beschreibung der elektrischen Doppelschicht für das Verständnis elektrochemischer Prozesse essentiell ist. Dafür ist die Untersuchung von Struktur und Dynamik der Grenzfläche zwischen Elektrode und Elektrolyt auf atomarem und molekularem Niveau mit experimentellen Methoden und theoretischen Modellen entscheidend. Ein Trend geht weg von rein wässerigen Elektrolyten hin zu organischen Lösungen, ionischen Flüssigkeiten und stark eutektischen Lösungsmitteln. Außerdem wurde deutlich, wie fruchtbar gerade in der Elektrochemie der interdisziplinäre Austausch ist. Die Metallabscheidung besitzt eine nicht zu unterschätzende Bedeutung in der Erforschung von neuen Materialien, vor allem auch im Bereich Energie und Energiespeicherung.

Das altehrwürdige Schloss Reisensburg und die durchweg hohe Qualität der Beiträge trugen zu einer überaus angenehmen Tagungsatmosphäre bei. Dabei waren Sprecher in ganz unterschiedlichen Karrierestufen vertreten, vom Master-Studenten über Doktoranden bis zu international renommierten Wissenschaftlern. Die Beiträge wurden meist ausführlich und intensiv diskutiert, manchmal auch noch unter den Stuckdecken des Speisesaals bei hervorragender Küche.

Die Postersitzung mit elf Beiträgen krönte den Abend des ersten Konferenztages. Beim Konferenzdinner am zweiten Abend des 3. Gerischer-Kolb-Symposiums musizierte die Harfenistin Mona Arnold zusammen mit Ludwig Kibler an Klarinette und Klavier mit Werken von Domenico Scarlatti, Camille Saint-Saëns, Paul Reade und Jules Massenet.

Das 3. Gerischer-Kolb-Symposium wurde unterstützt und gefördert von der Deutschen Bunsen-Gesellschaft für Physikalische Chemie (DBG), der Deutschen Forschungsgemeinschaft (DFG), dem Fonds der Chemischen Industrie (FCI), der *International Society of Electrochemistry* (ISE) und der Universität Ulm.

Ein besonderer Dank gilt dem Team vom Schloss Reisensburg und Frau Diemut Magon vom Institut für Elektrochemie der Universität Ulm für die Unterstützung bei der Organisation und Durchführung dieser internationalen Bunsen-Diskussionstagung. Man darf sich auf das 4. Gerischer-Kolb-Symposium in drei Jahren freuen.

Dr. Ludwig A. Kibler und Prof. Dr. Timo Jacob
Institut für Elektrochemie, Universität Ulm
Albert-Einstein-Allee 47, D-89081 Ulm
nawi.ec@uni-ulm.de

Thomas Leichtweiß, Adrian Schürmann

Solid-State Batteries VI: An International Bunsen Discussion Meeting

From Fundamentals to Application

November 13 to November 15, 2024, in Frankfurt am Main

The 6th International Bunsen Discussion Meeting on Solid-State Batteries took place in Frankfurt, Germany on November 13-15, 2024, and followed the very successful series of conferences held at Frankfurt House of Mobility and Logistics since 2014.

Around 230 participants discussed the status, progress, and latest trends in solid-state batteries (SSB). While conventional liquid electrolyte-based batteries slowly reach their limits, SSB attract growing interest for their expected stability, safety, and the intrinsic separator function of solid electrolytes. The latter may enable the use of lithium metal anodes thereby raising hope for a boost in battery capacity. However, despite the promises, many transport-related, interfacial, and chemo-mechanical challenges still need to be solved. In a broad community effort between computational scientists, experimentalists, and engineers from both academia and industry, different materials classes for anode, cathode and solid electrolyte are currently being explored and the remaining challenges for industrialization are being addressed. This meeting series fosters collaboration between leading experts from a wide range of fields, including physical chemistry, electrochemistry, materials science, solid-state physics, and engineering. By bringing together researchers from academia, research institutes, and industry, the forum stimulates an intensive exchange on the theoretical and practical limitations of SSBs.

The audience enjoyed a number of invited talks covering *Efforts from Semi-Solid to All Solid Lithium Batteries Via in situ Solidification Technologies* (Hong Li, Beijing, CN); *Columnar Si Anodes for Sulfide-Based All-Solid-State-Batteries* (Holger Althues, Dresden, DE); *Cutting Edge Research: An Introduction to CATL 21C Lab* (Ulderico Ulissi, Ningde, CN); *Ductile Super-Ionic Conductors for All-Solid-State Lithium Batteries* (Linda F. Nazar, Waterloo, CA); *Understanding the Evolution of Anode Materials and Interfaces in Solid-State Batteries* (Matthew T. McDowell, Atlanta, US); *Impact of Particle Size Distribution and Densification on the Development of Solid-State Pouch Cells* (Daniel Rettenwander, Trondheim, NO); *Hybrid Material Concepts and Benchmarking Solid-State Battery Performance* (Nella M. Vargas-Barbosa, Bayreuth, DE); *Chloride Electrolytes: A Perspective on Structure, Ion Conduction, Reactivity, and Cell Performance* (Raphaële Clément, Santa Barbara, US); *Challenges of All Solid State Battery for EV Application* (Koichiro Aotani, Yosuka, JP); *Cathode and Anode Interfaces in a Lithium-Anode Ceramic-Electrolyte Battery* (Peter G. Bruce, Oxford, UK); *Solid Electrolytes: From Mine to Cell* (Christoph Hartnig, Frankfurt, DE).

The invited talks were complemented by contributed talks from national and international researchers, including a significant number of early-career scientists and industry professionals. Additionally, over 120 contributed posters were presented.

Members of this year's scientific committee were Jürgen Janek (JLU Giessen), Wolfgang Zeier (University Muenster), Sabrina Zellmer (Fraunhofer IST) and Jeff Sakamoto (University of California). Additional information can be found at http://solid-state-batteries.net/ or requested from the conference organizers under info@lama.uni-giessen.de.

The conference series has been made possible by significant support from industry but also from the Deutsche Bunsen-Gesellschaft (DBG) and the Fonds of the Chemical Industry (FCI). The conference series is expected to return in 2026.

Participants of the 6th SSB Conference in the lecture hall of the HOLM in Frankfurt. Copyright: DBG/Weber

Poster session of the 6th SSB Conference. Copyright: JLU Gießen/Leichtweiß

Dr. Thomas Leichtweiß, Dr. Adrian Schürmann
Justus-Liebig-Universität Gießen
thomas.leichtweiss@lama.uni-giessen.de
adrian.schuermann@lama.uni-giessen.de

Ralf Ludwig

Dirk Guldi mit der Robert-Bunsen-Vorlesung ausgezeichnet

Prof. Dr. Dirk Michael Guldi von der FAU Erlangen-Nürnberg wurde am 5. November 2024 mit der Robert-Bunsen-Vorlesung ausgezeichnet. An der Universität Heidelberg, der wissenschaftlichen Heimat des Namenspatrons des Preises und unserer Gesellschaft, sprach Dirk Guldi zum Thema: „Towards Adaptive Light Capture, Conversion, and Storage“. Organisiert wurde die gut besuchte Veranstaltung von Petra Tegeder aus dem Physikalisch-Chemischen Institut und Felix Deschler, dem Vorsitzenden der Chemischen Gesellschaft zu Heidelberg. Die Laudatio hielt der Erste Vorsitzende der Deutschen Bunsen-Gesellschaft, Ralf Ludwig, die hier abgedruckt wird:

"Liebe Chemische Gesellschaft zu Heidelberg, liebe Anwesende,

es ist mir eine große Ehre und Freude, Dirk Guldi heute für seine herausragenden wissenschaftlichen Leistungen mit der Robert-Bunsen-Vorlesung 2024 auszuzeichnen.

Dirk Guldi begann seine Laufbahn in Köln, wo er Chemie studierte und 1990 promoviert wurde. Nach einem Jahrzehnt als Professor am Notre Dame Radiation Laboratory/USA, nahm er 2004 einen Ruf an der Friedrich-Alexander-Universität Erlangen-Nürnberg an.

Dirk Guldis wissenschaftliche Aktivitäten umfassen den Entwurf, die Entwicklung, die Synthese, die Analyse, die mechanistische Untersuchung und Modellierung neuartiger Materialien, die sich in besonderer Weise für die Energiewandlung und -speicherung eignen.

Der Fokus seiner Forschungsarbeiten liegt dabei auf nanoskalig strukturierten Materialien, die er mit komplexen, hochmodernen Methoden der zeitaufgelösten Spektroskopie und der nanoskaligen Strukturaufklärung untersucht, um damit neue Einblicke in die Struktur-Dynamik-Beziehungen auf molekularer Ebene zu gewinnen.

Exemplarisch möchte ich dafür drei Beispiele nennen:

In einer Vielzahl von hochkarätigen spektroskopischen Arbeiten konnten Dirk Guldi und sein Team die Mechanismen zugrundeliegender Prozesse der Singulett-Fission und Triplet-Triplet Upconversion verstehen und quantifizieren. Untersucht wurden organische Moleküle, Polymere und Nanomaterialien. Wichtig ist Dirk Guldi nicht nur exzellente Grundlagenforschung, sondern auch immer die Anwendung. Ziel ist hier, die Wirkungsgrade von Solarzellen durch Multiplikation von Ladungsträgern stetig zu verbessern.

Zu den Arbeitsfeldern von Dirk Guldi gehört auch die Untersuchung von Ladungstransferreaktionen in Porphyrin-basierten Architekturen. Hier reicht der Kanon von der Strukturaufklärung, der Untersuchung der Licht-induzierten Dynamik auf einer Zeitskala zwischen Femtosekunden und Millisekunden bis hin zur angewandten Materialwissenschaft. So konnte Dirk Guldi Triaden- und Tetraden-Strukturen identifizieren, die langlebige ladungsseparierte Zustände aufweisen – bis in den Sekundenbereich hinein, und sich besonders für den Einsatz in der Photokatalyse eignen.

Mit der kontrollierten Herstellung und Charakterisierung von Porphyrinoid-basierten Nanomaterialien sowie deren Assemblierung auf Oberflächen hat Dirk Guldi zudem das Tor zu elektronischen und optoelektronischen Anwendungen der maßgeschneiderten Strukturen in der molekularen Elektronik aufgestoßen.

Seine Studien über die ablaufenden Energie- und Ladungstransferprozesse in Kohlenstoff-Nanoröhren und Kohlenstoffallotropen liefern neues Anwendungspotential in der Elektronik, Katalyse und Energiegewinnung.

Dahinter verbirgt sich ein Konzept. Dirk Guldi bündelt die Methoden der modernen physikalischen Chemie, um grundlegende Forschungsfragen zu beantworten, aber auch um Anwendungspotenziale aufzuzeigen und auszuschöpfen.“

Von links nach rechts: Prof. Dr. Ralf Ludwig, Erster Vorsitzender der DBG 2023/2024, Prof. Dr. Dirk Guldi, Preisträger, Prof. Dr. Petra Tegeder, DBG-Vertrauensdozentin, Prof. Dr. Felix Deschler, Chemische Gesellschaft zu Heidelberg. Copyright: Universität Heidelberg/Liebscher.

Prof. Dr. Ralf Ludwig
Erster Vorsitzender der DBG 2023/2024
ralf.ludwig@uni-rostock.de

Eckart Hasselbrink, Sebastian Schlücker

Zellner-Wissenschaftspreis 2024 für Physikalische Chemie an der Universität Duisburg-Essen

An der Universität Duisburg-Essen (UDE) wurde im Sommersemester 2024 im Rahmen einer GDCh-Festveranstaltung zum dritten Mal der Zellner-Wissenschaftspreis für Nachwuchs-Forscherinnen und -Forscher in der Physikalischen Chemie vergeben. Die diesjährige Preisträgerin ist Frau Dr. Viktorija Glembockyte. Sie hat herausragende, innovative Beiträge zur Entwicklung hochempfindlicher optischer Biosensoren durch eine Kombination von Einzelmolekülfluoreszenzmikroskopie und DNA-Nanotechnologie geleistet – mit Arbeiten in *Nature Communications*, *Angewandte Chemie* und *Advanced Materials*. Durch die Integration von diagnostischen Assays in DNA-Nanoantennen lassen sich die Fluoreszenzsignale mehrere hundertfach verstärken. Diese optische Methode ist so empfindlich, dass sogar einzelne DNA-Moleküle auf einem Batteriebetriebenen Smartphone-Mikroskop detektiert werden können. Mit diesem innovativen Ansatz zum mobilen Vor-Ort-Nachweis kann beispielsweise eine Antibiotikaresistenz nachgewiesen werden, so dass sich hieraus ein enormes Anwendungspotential ergibt. Frau Dr. Viktorija Glembockyte hat ihre ausgezeichneten Arbeiten in der Physikalischen Chemie der Ludwig-Maximilians-Universität (LMU) und dem Center for Nanoscience (CeNS) München durchgeführt. Seit Oktober 2024 leitet sie die Forschungsgruppe „Single Molecule Sensing“ am Max-Planck-Institut für medizinische Forschung in Heidelberg.

Gestiftet wurde der mit 3.000 EUR dotierte Preis vom Essener Atmosphärenforscher Prof. Dr. Dr. h.c. Reinhard Zellner, der dazu eine Stiftung gegründet hat. Reinhard Zellner war von 1991 bis 2010 C4-Professor für Physikalische Chemie und von 2010 bis 2018 Senior-Professor an der Fakultät für Chemie. Seine Forschungsthemen waren laserspektroskopische Untersuchungen der Kinetik von fundamentalen Prozessen in der Atmosphäre in der Gasphase sowie heterogenen Prozessen in und an Aerosolen. Prägend hat er in den 1990ern das Deutsche Ozonforschungsprojekt in der Arktis und von 2008 bis 2015 das DFG-Schwerpunktprogramm „Biological responses to nanoscale particles“ geführt. Er hat seine Expertise in zahlreichen Gremien des BMBF und der EU sowie von DECHEMA und GDCh eingebracht.

Der Vortrag der Preisträgerin mit dem Titel „Nanoscale Tools for Sensing Single Molecules” fand am 12. Juni 2024 im Rahmen eines GDCh-Festkolloquiums statt. Der anschließende Empfang wurde freundlicherweise von *Evonik Industries* finanziell unterstützt. (von links: *Laudator Prof. Claus Seidel, Preisstifter Prof. Reinhard Zellner, Preisträgerin Dr. Viktorija Glembockyte, Prof. Sebastian Schlücker, Prof. Eckart Hasselbrink).*

Prof. Dr. Sebastian Schlücker
Physikalische Chemie, Universität Duisburg-Essen
Universitätsstr. 5, D-45141 Essen
sebastian.schluecker@uni-due.de

Prof. Dr. Eckart Hasselbrink
Physikalische Chemie, Universität Duisburg-Essen
Universitätsstraße 1, D-45141 Essen
eckart.hasselbrink@uni-due.de

Hellmut Eckert, Paul Heitjans, Andreas Heuer, Joachim Maier, Bernhard Roling, Monika Schönhoff

Die Bunsen-Gesellschaft für Physikalische Chemie und die internationale wissenschaftliche Community trauern um ihr Mitglied

Prof. Dr. Klaus Funke,

der am 21. Oktober 2024 im Alter von 79 Jahren verstorben ist.

Klaus Funke, geboren am 16. Dezember 1944, studierte in Göttingen Physik und promovierte dort 1970 unter Wilhelm Jost über die Kationen-Leitfähigkeit in Ionenkristallen. Nach einem Postdoktorandenaufenthalt am Institut Laue-Langevin in Grenoble habilitierte er sich 1976 in Göttingen in Physikalischer Chemie. 1979 folgte er einem Ruf an die Universität Hannover. Dort leitete er die Abteilung für Elektrochemie und war bis 1988 Mitglied im DFG-Sonderforschungsbereich „Lokale Teilchenbewegung, Transport und chemische Reaktion in Ionenkristallen“ (Gründungssprecher Hermann Schmalzried). 1985 übernahm er als Nachfolger von Ewald Wicke den Lehrstuhl am Institut für Physikalische Chemie in Münster, den er bis zu seiner Emeritierung innehatte.

Klaus Funke hat sich in großer Tiefe und Breite mit der Ionendynamik in Elektrolyten beschäftigt, einem Kernaspekt bei der Wirkungsweise von Batterien. Besondere Aufmerksamkeit haben seine Arbeiten zum Verständnis der dynamischen Prozesse in festen Ionenleitern auf ganz unterschiedlichen Zeitskalen erlangt. Neben exzellenten experimentellen Arbeiten, die auf einer Vielzahl von speziell entwickelten Methoden basierten (u.a. Leitfähigkeitsspektroskopie über 17 Frequenzdekaden), hat Klaus Funke mit großer Leidenschaft Modelle entwickelt, die eine mechanistische Interpretation der Beobachtungen ermöglichen.

Als besondere Auszeichnung für seine Forschungsarbeiten erhielt Klaus Funke 1980 den Walter-Schottky-Preis der Deutschen Physikalischen Gesellschaft sowie 1997 die Wilhelm-Jost-Gedächtnismedaille und -Vorlesung. Als Erster Vorsitzender der Bunsen-Gesellschaft 2003 bis 2004 hat er die Physikalische Chemie auf nationaler Ebene prominent vertreten. Zudem hat Klaus Funke als Initiator und Sprecher des DFG-Sonderforschungsbereichs „Ionenbewegung in Materialien mit ungeordneten Strukturen – vom Elementarschritt zum makroskopischen Transport“ eine wichtige Basis für die aktuelle Batterieforschung geschaffen.

Über viele Jahre war Klaus Funke Vorsitzender des Wissenschaftlichen Beirats des Stuttgarter Max-Planck-Instituts für Festkörperforschung und hat in dieser Funktion stets die Bedeutung des Ionentransports hervorgehoben. Die internationale Solid State Ionics Community hat ihm neben seinen wissenschaftlichen Errungenschaften viel zu verdanken. Er war von 2007 bis 2009 Präsident der International Society for Solid State Ionics (ISSI) und einer der Gründungsväter des gleichnamigen Journals.

Der direkte persönliche Austausch war Klaus Funke besonders wichtig. Mit seiner ansteckenden Begeisterung für die Forschung hat er die Atmosphäre im Institut und zwischen den Münsteraner Fachbereichen Physik und Chemie sehr positiv geprägt und auf dem internationalen Parkett waren seine druckreif ausgearbeiteten Vorträge eine wiederkehrend inspirierende Attraktion. Seine persönlichen wissenschaftlichen Kontakte pflegte er intensiv. Hier ist besonders Malcolm Ingram aus Aberdeen zu nennen, mit dem er seine Begeisterung für springende Ionen teilte, wobei bei mittäglichen Diskussionen schon mal Salz- und Pfefferstreuer zur Demonstration herhalten mussten.

Generationen von Studierenden erinnern sich an seine hervorragend gestalteten Vorlesungen der Physikalischen Chemie, die er stets aus dem Kopf, d.h. ohne Manuskriptvorlage, direkt an der Tafel entwickelte und mit anschaulichen Skizzen sowie mit interessanten, teils tiefsinnigen Anekdoten anreicherte. Gerne erinnern wir uns auch an seine besondere Vorliebe für Wort- und Zahlenspiele (Palindrome und Limericks).

Zu Klaus Funkes wissenschaftlichem Vermächtnis zählen ca. 150 Publikationen sowie vier habilitierte und etwa 60 promovierte Wissenschaftler. Die Atmosphäre in seiner Arbeitsgruppe war gekennzeichnet von gegenseitigem Respekt und der Freiheit, sich intensiv mit grundlegenden wissenschaftlichen Fragestellungen zu beschäftigen und hierbei eigene Ideen und Forschungsansätze zu verfolgen.

Nach seinem Eintritt in den Ruhestand hat er sich noch intensiver seinem wissenschaftlichen Hobby, der Astronomie, gewidmet und in diesem Feld auch publiziert.

Unser tiefes Mitgefühl gilt seiner Frau Margit und seinen beiden Töchtern Kirsten und Cornelia.

Wir werden sein Andenken stets in Ehren halten und lassen ihn mit einem Gedicht aus seiner Feder noch einmal zu Wort kommen.

Science

You only live twice,
or so it seems,
once in your life
and once in your dreams.

But somewhere between
your life and your dream
there is a kind
of third state of mind.

It takes you on wings
and makes you see things.
Pictures arise
in front of your eyes.

They strike you like thunder
and leave you in wonder.
Surprise, revelation:
you see the equation.

You're lucky if you
can cherish a few
moments like this,
since each is a bliss.

K. Funke

ZITATBOX

Sergio Bambaren

*„Vielleicht bedeutet Liebe auch lernen,
jemanden gehen zu lassen,
wissen, wann es Abschied nehmen heißt.
Nicht zulassen, dass unsere Gefühle dem im Weg stehen,
was am Ende wahrscheinlich besser ist für die,
die wir lieben."*

Quelle: https://www.zitate7.de/autor/Sergio+Bambaren/

Mark Twain

„Weine nicht, weil es vorbei ist, sondern lache, weil es so schön war."

Arthur Schopenhauer

„Ich glaube, dass wenn der Tod unsere Augen schließt, wir in einem Lichte stehen, von welchem unser Sonnenlicht nur der Schatten ist."

Ohad Kamin

„Das Leben ist kurz. Wenn Sie die Entscheidung treffen, welchen Weg sie einschlagen, sollten Sie sich zuerst über die Dinge Klarheit erschaffen, die Sie tun können. Wählen Sie von diesen die aus, die Sie tun wollen. Und von diesen dann die, die Sie wirklich tun wollen. Finden Sie schließlich die Dinge, die Sie wirklich, wirklich tun wollen – und tun Sie sie."

Erich Fromm

„Mit der Geburt wird der Mensch... in eine Situation hinein geschleudert, die nicht festgelegt, sondern ungewiss und offen ist. Nur in Bezug auf die Vergangenheit herrscht Gewissheit, und für die Zukunft ist nur der Tod gewiss."

Quelle: https://www.sinndeslebens24.de/zitate-ueber-den-tod-die-wichtig-sind-fuer-das-leben

Johann Wolfgang von Goethe

"Was man tief in seinem Herzen besitzt, kann man nicht durch den Tod verlieren."

Dietrich Bonhoeffer

Je schöner und voller die Erinnerung, desto schwerer ist die Trennung. Aber die Dankbarkeit verwandelt die Erinnerung in eine stille Freude. Man trägt das vergangene Schöne nicht wie einen Stachel, sondern wie ein kostbares Geschenk in sich.

Quelle: https://www.trauersprüche.de/weltlich

Geburtstage im Februar 2025

Günter Tovar, Prof. Dr.

Eckhard Spohr, Prof. Dr.

Franz-Georg Simon, Prof. Dr.

Michael Buback, Prof. Dr.

Cornelius Zetzsch, Prof. Dr.

Alfred Blume, Prof. Dr.

Dietrich Menzel, Prof. Dr.

Geburtstage im März 2025

Volker Kapune

Jürgen Fleig, Prof. Dr.

Martin Hartmann, Prof. Dr.

Manuel Galán-Vioque, Dr.

Klaus Kern, Prof. Dr.

Markus Winterer, Prof. Dr.

Hans-Gerd Löhmannsröben, Prof. Dr.

Wolfram Vogelsberger, Prof. Dr.

Klaus Heinrich Homann, Prof. em. Dr.

Das Bunsen-Magazin dokumentiert Geburtstage der DBG-Mitglieder in Fünfjahresschritten – beginnend mit dem 60. Geburtstag. Mitglieder, die keine Veröffentlichung ihres Geburtstags wünschen, teilen dies bitte der DBG-Geschäftsstelle mit: geschaeftsstelle@bunsen.de.

Neuanmeldungen zur Mitgliedschaft

Ruben Cruz
Noah Oriol Evers
Rico Friedrich, Dr.
Mathis Julian Gölz
Ibrahim Sadiek, Dr.
Felix Drexlmeier
Lina Möllmann
Marius Gerlach, Dr.

Verstorben

Klaus Funke, Prof. Dr.
im Alter von 79 Jahren
Wolfgang Wiebauer, Dr.
im Alter von 78 Jahren

Veranstaltungen

Deutsche Bunsen-Gesellschaft

Bunsen-Tagung 2025
Physical Chemistry of the Climate and the Atmosphere
17.- 19. März 2025, Leipzig
www.bunsentagung.de

Bunsen-Tagung 2026
Properties and Processes under Confinement
30. März-01. April 2026, Dresden

Weitere Veranstaltungen

51st German Liquid Crystal Conference 2025
26.-28. März 2025, Göttingen
https://www.uni-goettingen.de/de/686467.html

IUPAC World Chemistry Congress 2025
14.-19. Juli 2025, Kuala Lumpur
www.iupac2025.org

flavors & fragrances 2025
22.–24. Juli 2025, Göttingen
www.gdch.de/flavorsfragrances2025

76th Annual Meeting of the International Society of Electrochemistry
07.-12. September 2025, Mainz
https://annual76.ise-online.org/

61st Symposium on Theoretical Chemistry
Exploring Energy Landscapes
22.-26. September 2025, Berlin
https://www.bcp.fu-berlin.de/en/stc2025/index.html

GDCh Science Forum Chemistry 2025
29.09.-01.10.2025, Karlsruhe
https://www.gdch.science/

Verschiedenes

Merck KGaA Darmstadt Germany Innovation Cup

The Innovation Cup is an initiative for post-graduate students on their way towards a PhD or postdocs in natural sciences, computer sciences, and business administration to attend a training program from 19-25 July 2025 in Darmstadt, Germany.
The Innovation Cup is designed to support the professional development of post-graduate students interested in the pharmaceutical, chemical and digital industry. Participants learn how R&D in the industry works by lectures from Merck managers and scientists. The students will also advance an idea to a full project plan with their teams. Teams will work on innovative projects in the areas of: Oncology, Neuroscience & Immunology, Drug Discovery, Green Chemistry, Digital Health, Neuro-inspired AI Inference Acceleration and Smart Manufacturing.
Postdocs and post-graduate students on their way towards a PhD in biology, chemistry, physics, medicine, biotechnology, computer sciences, data sciences, biochemistry, pharmacy, engineering or related fields are invited to apply. In addition, advanced MBA students or recent MBA graduates with an interest in the pharmaceutical, chemical and digital business and a background in natural sciences or computer sciences are also eligible. All travel, food and accommodation expenses are paid by Merck KGaA Darmstadt.
Applications for the 2025 Innovation Cup close 31 January 2025 and can be submitted here:
https://innovationcup.merckgroup.com or https://innovationcup.emdgroup.com

Deutsche Bunsen-Gesellschaft
für physikalische Chemie

Einladung zur Mitgliederversammlung der

Deutschen Bunsen-Gesellschaft für physikalische Chemie e.V. (DBG)

Gemäß § 10 der DBG-Satzung berufen wir hiermit die Mitgliederversammlung 2025

unserer Gesellschaft für

Montag, 17. März 2025, 13.30 Uhr

nach Leipzig ein.

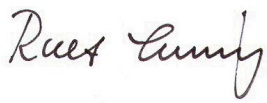
Die Mitgliederversammlung findet statt im Hörsaal Süd 2, Campus Jahnallee, Haus 1,

Universität Leipzig, Jahnallee 59, 04109 Leipzig.

Tagesordnung

1. Bericht des Vorstandes über das abgelaufene Geschäftsjahr
2. Feststellung der Jahresrechnung, Bericht des Schatzmeisters über den Jahresabschluss und über das laufende Geschäftsjahr
3. Entgegennahme und Genehmigung des Berichts der Rechnungsprüfer:innen
4. Entlastung des Vorstandes und der Geschäftsführung
5. Vornahme der erforderlichen Wahlen
6. Festsetzung des Jahresbeitrages
7. Beschlussfassung über Ort und Zeit der nächsten Hauptversammlungen (Bunsen-Tagungen)
8. Beschlussfassung über die Satzungsänderungen in §1, §2, §3, §4, §5, §6, §7, §8, §9, §10, §11, §12, §13, §14, §15 und §16 (Anlagen: www.bunsen.de/mitgliederversammlung)
9. Beschlussfassung zur Ermächtigung des Vorstandes zu Satzungsanpassungen entsprechend behördlicher Vorgaben
10. Beschlussfassung über eingegangene Anträge
11. Verschiedenes

Diese Einladung richtet sich nur an Mitglieder der DBG. Anträge aus der Mitgliedschaft (TOP 10) müssen gemäß §10 Abs. 4 der DBG-Satzung einschließlich einer kurzen Begründung mindestens vier Wochen vor der Mitgliederversammlung, d.h. spätestens am 17. Februar 2025, dem Ersten Vorsitzenden vorliegen. Anträge sind fristgerecht mit entsprechender Begründung an den Ersten Vorsitzenden, geschaeftsstelle@bunsen.de, zu senden.



Prof. Dr. Ralf Ludwig
Erster Vorsitzender der DBG 2023/2024
Zweiter Vorsitzender der DBG 2025

Prof. Dr. Robert Franke
Zweiter Vorsitzender der DBG 2024
Erster Vorsitzender der DBG 2025-2026

Info und Anlagen zum Tagesordnungspunkt 8 „Beschlussfassung über Satzungsänderung […]“

Die Satzungsänderung war bereits Inhalt der DBG-Mitgliederversammlung 2023. Aufgrund formaler Fehler in der Tagesordnung und Einladung zur Mitgliederversammlung ist die Satzungsänderung erneut Beschlusspunkt der Mitgliederversammlung. Zudem haben das Finanzamt und das Vereinsregister Frankfurt noch Punkte angemerkt, die rechtlich relevant sind und in der Satzung geändert werden müssen. Einen Entwurf der neuen Satzung sowie Dateien, in der Sie alle Änderungen nachverfolgen können, stellen wir Ihnen wegen des Umfangs online auf www.bunsen.de/mitgliederversammlung zur Verfügung. Bei Fragen melden Sie sich bitte bei der DBG-Geschäftsstelle per E-Mail (geschaeftsstelle@bunsen.de) oder telefonisch (069-7917 336, 09:00-12:30 Uhr).