

Volume 54
Edition 2



ACID

Snow Formation

How snowflakes get their unique shape

Amsterdams
Chemisch
Dispuut

Working as a Junior Lecturer

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From the Editor

Dear reader,

This edition of the ACiD marks the end of an era, and the beginning of a new one. About 3.5 years ago, I took over the designing portion of our lovely ACD magazine and taught myself how to work with Adobe InDesign and Photoshop. The committee gave me their trust and allowed me full creative freedom, and so the template for the ACiD as you know it now was born. Many ACD'ers are probably familiar with my work in some way or another, as I have been responsible for the designs of the ACiD of the last 3.5 years, all three editions of the first year magazine and together with Marit the Almanak to celebrate the 75th birthday of the ACD. But all good things must end and the time had come for me to find a successor. Fenna has helped me out with the design of this and last edition and starting from the next one, she will take it over completely. Although I am sad to say goodbye, I am also excited to see what creations Fenna's creativity will bring us. However, this goodbye is not final yet, as I will still be writing some articles for the ACiD. As usual, we hope you have fun reading this edition.

On behalf of our entire editing team,

Myrthe Zwart

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From the Chair

Dear ACD'ers,

The past months were filled with fun and interesting activities. We started November with a thrilling Halloween party with our brother association SABA. This was followed by another kind of party: the ACD birthday! The 77th birthday of our loved association was celebrated with free cake in both member rooms and the board who had their board meeting with party hats on! Later that week we all celebrated once again during the Dies borrel.

All committees worked hard and organized plenty of activities. For example, the first years had a high-tea speed dating activity hosted by the EJC and the MAC organized a glow-in-the-dark mini-golf activity. Both activities were well attended and the perfect opportunity for the students to get to know their peers during this first semester. We also got activities organized by the ACTIE!, CWAL, LEC and Chemunity, and I was very pleased to see so many ACDers at all of these events. We ended the year in style with the amazing cooking skills of the KoCo during the AChristmasDiner.

My personal favorite was the first VU borrel the ABC organized along with another brother association STORM. During this chemical-themed borrel, we took "some" very tasty shots out of reaction tubes. Another favorite was the V.O.D.K.A. borrel. I invited some board members from our sister association the Chemische Binding from Groningen and they actually came all the way just for our borrel (see the picture)!

I hope everyone had a great holiday and enjoyed their time with family and/or friends! I am looking forward to what 2023 has to bring and how filled it will be with the most fun ACD events. I hope to see you all there!

Love,
Your chair
Fay Heemskerk



Het Wel en Wee van de OC

Evelien van Erven

Dear reader,

In the last column I introduced myself as a new member of the programme committee (OC) and the new writer of this column, and I mentioned that I was being taught my responsibilities and how to execute them as best as I could. Since then, there has been the second meeting of the committee, a training for new members, and an informal meeting with other programme committees in which we discussed our annual plans, problems we ran into and how we (plan to) tackle them.

One problem which I heard surprisingly often is the topic of new curricula that we have in the bachelor now. Generally, we agreed that the best way to deal with the problems arising in the first cohorts where they are implemented is by keeping an open ear to feedback. To increase the response of course evaluations (one of our main sources of information), which currently tends to be somewhere around 30%, the committee has decided to return to paper evaluations as was customary before COVID - it has been proven this leads to double or even triple the response rates we have currently. It will also likely reduce the amount of pushy emails you currently get after your exams. :)

Now for a quick update on matters discussed last time and an introduction of new points:

- The resits for old curriculum bachelor students were discussed during our last meeting, and it has been decided to solve problems as they arise. If additional resits or different examination methods are deemed necessary when students fail their resits, we will tailor solutions to the problem instead of

thinking of general ones beforehand. Don't worry: you will always be able to get your credits.

- UvA Q and its replacement: no news as of right now.
- Physics for Chemical Sciences and the expensive textbook required: the course coordinator is still searching for a solution.
- GLASS and the 42 EC limit in course registration: we are firmly against this implementation, and believe that it should be in the OER-A (which it is currently not) if it is supposed to be an enforced rule. New rules like this should be approved by the faculty student council (FSR), and we have informed them that they have our support in attempting to get this rule revoked.

Lastly, we are working on a new Master's track in biochemistry, to provide a better connection to this new track in the bachelor. Célia Fonseca Guerra, the Master's programme director, is working hard on coordinating this new implementation, and we are given plenty of insight and comment options by her. More information on this will follow from the standard sources, but I just wanted to mention it here as it is quite an exciting prospect.

Plenty of information, and because I have a hard word limit, I really should end it here. As always, I'll keep you posted on updates arising to these matters and anything else I deem important in future columns.

OC mail: ocs-science@uva.nl

OC page: <https://student.uva.nl/onderwerpen/opleidingscommissie>

Year Overview 2022

Jiri Sanramat

January

3 – Peter Wright becomes World Champion Darts after defeating Michael Smith 7 – 5.

10 – Kabinet Rutte IV starts. VVD, CDA, D66, and CU form the coalition.

15 – The Voice of Holland is cancelled after accusations of sexual harassment.

February

4 – The Olympic Winter Games start in Peking.

20 – End of the Olympic Winter Games, the Netherlands finished 6th overall with 8 gold medals, 5 silver medals, and 4 bronze medals.

24 – Russia invades Ukraine.

March

3 – Nuclear power plant Zaporizja in Ukraine is invaded, this is the first time that a nuclear power plant has been invaded.

16 – Russia is disbarred from the council of Europe.

16 – The gemeenteraadsverkiezingen are held.

April

24 – Emmanuel Macron is reelected as president of France.

May

11 – AFC Ajax becomes champion of the Eredivisie with a 5 – 0 win from SC Heerenveen.

24 – School shooting at an elementary school in Texas, USA.

June

24 – Supreme Court of the United States overruled 'Roe v. Wade,' meaning that abortion laws are not regulated federally anymore.

25 – Terrorist attack on a gay club in Oslo, Norway.

July

1 - The Tour de France starts in Copenhagen.

8 – Former prime minister of Japan, Shinzo Abe, is shot.

24 – End of the Tour de France, Jonas Vingegaard wins.

August

8 – The FBI searches the house of former president of the USA Donald Trump, based on the suspicion of him having classified documents at home.

September

8 – Queen Elizabeth of the United Kingdom passes away, her son Charles II becomes the new King of the UK.

October

9 – Max Verstappen becomes Formula One World Champion for the second time at the GP of Japan, with 4 races left.

30 – Tribulation on Halloween in Seoul, South Korea, resulting in the death of 153 people.

November

8 – The 8 billionth living person is born

20 – 22th World Cup Football starts in Qatar

December

9 – Oranje, after a controversial quarter final game, is eliminated from the World Cup.

19 – World Cup Final between Argentina and France, the last international match of Lionel Messi.

Working as a Junior Lecturer

From Taking Exams to Making Exams

Rianne van Diest

During your study, you might wonder sometimes (or very often) where you'll end up after obtaining your degree. This interview will give you an insight in one of the many career possibilities: becoming a junior lecturer! I talked with Jesper Ruiter, who is working as a junior lecturer at the VU since September.

Study and career

Jesper followed both his bachelor and master in chemistry at the UvA/VU. In the bachelor, he did the 'orientation in education' project, in which he experienced teaching at a high school. Although he liked the teaching, Jesper has a great passion for chemical research as well, so for the master, he chose the research variant of the analytical sciences track. Next to his internship, he has worked as teaching assistant for the first-year bachelor course Molecular Analysis.

After the master, he was not completely sure what to do. He knew he liked teaching, but also doing research, so he applied for a PhD position. The group was very positive about his application, but during the interview, they came up with a surprising suggestion. Apparently, the feedback from students of the Molecular Analysis course on Jesper was very positive. The group had an open position for a junior lecturer, and they thought that Jesper would be very suited for this role. Since Jesper had enjoyed the teaching as well, he agreed to take this position. He has a contract for one year now, which he can use to figure out if he wants to continue his career in teaching, or pursue a PhD after all. Until now, he really likes working as a junior lecturer.

Working as a junior lecturer

When I asked about Jesper's day at the start of this interview, he told me that he was designing exams for one of the courses that he is teaching.



Now, that's something else: from being a student and taking exams, to teaching students and making exams! Besides, Jesper teaches the lectures and seminars of various courses. For the lectures, there are old slides available, but he gives them his own spin, and tries to make them more interactive by adding mini-quizzes. He has a lot of contact with the course coordinators, and together they think about the course design and how to improve this. Outside the lectures, he answers questions from students via mail, or they can stop by in his office. In addition, Jesper is involved in the design and testing of new lab practicals for the students. Lastly, he keeps track of the registration of student projects within his group.

Furthermore, Jesper follows the University Teaching Qualification program (UTQ, known as

BKO in Dutch). This two-year program focuses on designing a course, or creating a safe and inclusive learning environment. Following this program is not required for his job, but it is a valuable certificate to have, as it will allow him to teach at the higher professional education programs (HBO) as well, or become a course coordinator.

What he likes most about his job? 'Talking about chemistry and getting paid for it!'. Jesper takes great joy from conveying his passion for chemistry to the students, and having nice discussions with them. He also tells that this is a large difference from teaching in high school. There, the theory is much less profound compared to the university, and in addition, not all students are interested in learning chemistry. In university, all students chose this degree, so they are motivated to learn more about the topic. There are no big aspects of his job that Jesper does not like, but he admits that grading exams and reports is always a tedious task. I think that everyone who has worked as a teaching assistant can agree with that...

For his job, Jesper has a lot of use from the chemical knowledge obtained in both his courses and his internships. Besides, he used to perform in the theatre during high school, and his experience with standing in front of large groups and connecting with the audience comes in handy. Moreover, he tells he can actually apply a lot of skills from the first-year course Academic Skills. He admits that he thought it was a boring course when he was a first-year student, but

now, he gets to apply all the tips on giving good presentations and constructing nice feedback. As I'm teaching the Academic Skills course myself, I obviously couldn't pass up this opportunity to emphasize that it is certainly a useful course. Jesper tells that he obtains additional useful skills from the UTQ program. It provides tricks for making a course more interactive, or lowering the threshold for students to answer questions during lectures.

Future and advice

At this moment, junior lecturer positions are contracts of a maximum of four years. Jesper wants to get his UTQ qualification at least, and he wants to use his time here to build up connections. Then, he could also switch to teaching at the HBO. If the contract would become permanent, and he still likes the work at that time, he would consider staying here as well. For students thinking about a job as junior lecturer, Jesper recommends to try out teaching at a high school with a minor teaching and as teaching assistant at university. In that way, you can experience if you like teaching in the first place, and see the difference between high school and university teaching jobs. These experiences helped him a lot in making his choice. Lastly, he thinks that you should always choose something that gives you joy. 'If you can't say that you like it for the full 100%, it might not be the job for you. It won't last you in the long run if you only like half of your job.'

Snow Formation

Janne van Asselt

It is winter again, so that means snow. Snow can be very annoying, like when your trains get cancelled. But nothing gives you more of a wintery feeling than snowflakes! Have you ever caught a snowflake and wondered how it got its distinctive shape? Each snowflake is shaped like a hexagon and has six-fold symmetry, but no two snowflakes are identical. Each one has its own unique shape. You might think that the formation of this structure is very complicated, but the chemistry behind it is actually quite simple!

Johannes Kepler also wondered how snowflakes got their shape, but at that time there was no atomic theory of matter yet.¹ He compared snow to honeycomb. If you zoom in on snow, the structure consists of hexagonal rings of six oxygen atoms. These rings all have six-fold symmetry, so this could explain the symmetry in snowflakes. But what is the cause of the six-sided oxygen rings? To answer this we will look at the water molecules. Due to the polarity and tetragonal shape of water molecules, the hexagon shape is the most stable formation. This formation is shown in Figure 1B. Here the water molecules form hydrogen bonds with 3 other molecules and the angles are not shifted a lot compared to its free form, as shown in Figure 1B. So the hexagon lattice is formed due to the properties of water.

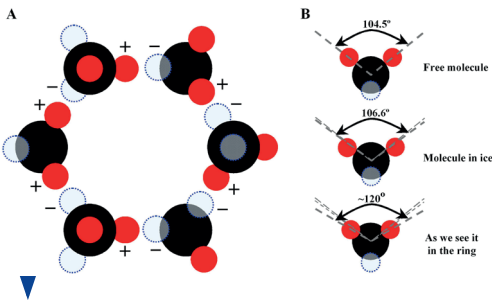


Figure 1: A. The electric forces between electrons and lone pairs force the water molecules in a hexagonal ring B. The angles of water as a free molecule compared to the angles in the ring.¹

That the internal lattice is hexagonal does not necessarily mean that the outside is a hexagon, but for snowflakes this is the case. To explain this, we'll take a look at Figure 2.¹ On the red lines, only one molecule of the hexagonal ring lies at the surface. Here the forces make that surface grow relatively slow. On the green lines two molecules from the ring lie at the surface, resulting in faster growth. As soon as molecules attach to these green faces, these also turn into red-faces (B). This eventually results in the hexagon shape (C).

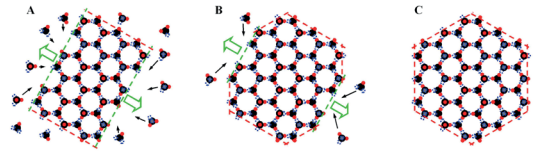


Figure 2: A. Hypothetical rectangle shape. The red dashed lines grow slow while green edges grow fast. B. As water molecules attach, the crystal forms new slow growing edges. C. As growth continues, the fast growing edges disappear resulting in a hexagon.¹

So now we know the cause of the hexagon shape. Let's look into the formation of the symmetric branches. Since the six corners of the hexagon stick out, they can collect water faster than the sides of the crystal.² This causes the branches to sprout. For a snowflake the conditions around it are almost constant, each branch grows at the same rate. How the branches grow differs per snowflake because it is dependent on the conditions. The temperature and humidity are the main factors that affect the shape. The temperature mainly determines whether the snow crystals will form plates or columns. This is shown in Figure 3. When the humidity is low, crystals will form slowly and into simpler forms. Higher humidity will form more complex crystals.

The most famous snowflake structure is the dendrite. This is the shape most of us picture when we think of a snowflake. The structure is formed at temperatures around -3°C , but at these conditions the crystals formed are small. At colder temperatures of -20 to -25°C larger dendrites are formed.

So, even though there are still some mysteries around how snowflakes are formed, we now know how they get their hexagon shape and six-fold symmetry. Next time you see a snowflake, you don't have to wonder how it was formed anymore.

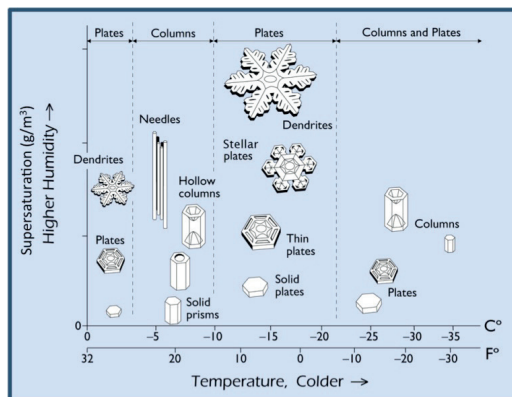


Figure 3: The morphology diagram of snow crystals.²

1. <https://www.storyofsnow.com/blog1.php/how-the-crystal-got-its-six>
2. <https://chalkdustmagazine.com/blog/snowflake-misteries-behind-symbol-winter/>



Interview with confidential advisers ACD

Get to know Jari Hoffmann and Siza Kuin and their perspectives on social safety

Anne-Fay de Jong

Social safety is always a very important topic, especially in social settings like activities of study associations. When you go from your safe cosy home to the university buildings for your classes, a sense of social safety is also preferable. The UvA and VU have confidential advisers, who you can contact after any undesired behaviour has occurred. The ACD has its own confidential advisers! I interviewed Jari Hoffmann and Siza Kuin to ask them about their job description and social safety.



What is your definition of social safety?

Social safety is about creating a safe and respectful environment for everyone, where anyone can express themselves in their own way without disrespecting others.

What is the role of confidential advisers?

Our role as confidential advisers of the ACD is different from those of universities or companies. For us, it is to be easily approachable for whatever may be on your mind, so you can just vent or be directed to the right people, as we possess the required knowledge. For the confidential advisers of the UvA, for example, they are more professional—better trained—and can only help after specific instances of undesired behaviour that had something to do with the UvA (for example that it occurred on UvA grounds).

What do you think is the importance of confidential advisers in general?

For me (Jari), it is important that anyone who is facing any problems will be heard. At least someone will be able to listen, and you won't have to face the consequences alone. I would say (Siza) in a more practical fashion that problems, within

the ACD or the UvA, get reported and do not stay unheard.

Why do you think it is important to have confidential advisers within the ACD?

(The active part of) the association is so small that gossip spreads very easily. It is important to have confidential advisers within the ACD so you can approach your issues in a more confidential way so that the gossip doesn't become or stay gossip.

Are all your conversations with ACD members strictly confidential?

Not all conversations are confidential because then we couldn't talk to anyone or participate in any activities of the ACD! Our conversations are only confidential when people approach us as confidential advisers, and we will mention that beforehand.

What do you think makes a good confidential adviser?

It is very important that a confidential adviser can separate their personal opinion from the conversations. As a confidential adviser of the

the structure of the association, however, one should not be too much involved with the “inner circle” of the association, such as (multiple) very active committees or the board for that matter—there should be a nice balance. Also, being open to everyone and being able to listen and talk to them is very important, especially to listen.

What do you get out of the experience of being a confidential adviser for the ACD?

What I (Siza) get out of this experience is the fulfilment of helping people and/or helping them understand where they can go and making them feel less alone. I learned (Jari) a lot about the topic of social safety when we did the course for becoming a confidential adviser of the ACD. Before the course I did not know much about it, and after I had lost some prejudices and learned that some aspects are more complicated than I thought.

Were you satisfied with the first social safety activity called Meet the Confidential Advisers?

What was the goal of that activity?

We were very pleased with the activity! It was held on the 8th of December and the turnout was alright. It was meant as a trial of such an activity, to see how we would do something like this. The idea was to bring social safety to everyone’s attention and have conversations about social safety within the association. One of the goals was that committee members and board members would think of this when organising activities for the ACD. The activity was more focused on everyone’s personal role in social safety within the association, but we also showed information about the confidential advisers. One of the UvA confidential advisers, Belle Jansen, was also present and we would like to thank her for her contribution, as she added a bit of professionalism to the activity.

What can other ACD- members do to favour and/or maintain social safety at the ACD?

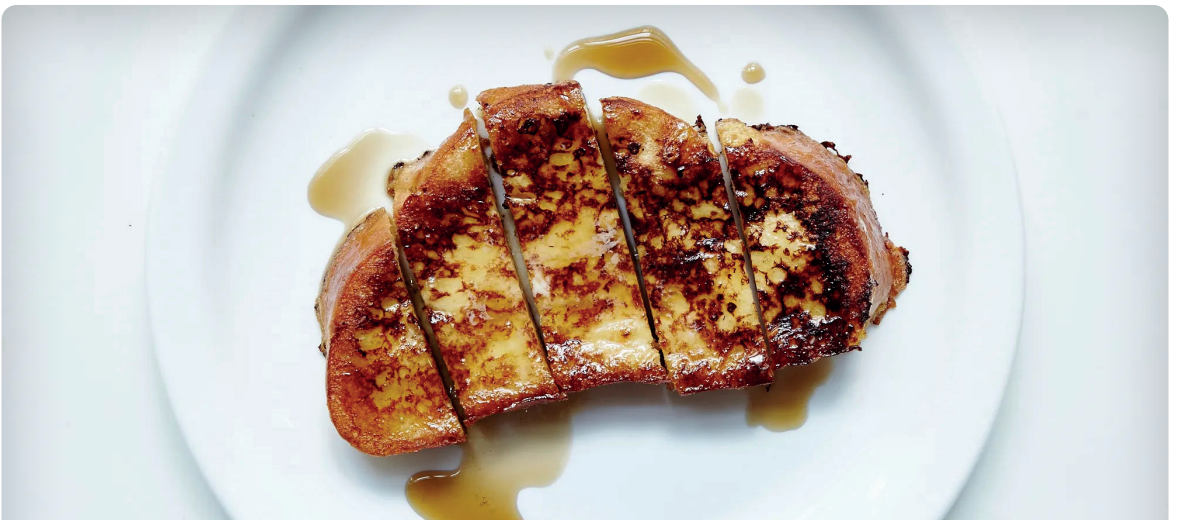
You should just be conscious of your surroundings. We talked a bit about it during the activity, but everyone is an active bystander, and you always have the option to do something. When you are conscious of this, you can create a socially safe environment. Everyone has an influence on social safety. So, in general, just try to be respectful.

Do you see any particular pitfalls for social safety in activities or other aspects of the ACD?

The one thing we have already touched upon is the gossip culture within the ACD. It easily occurs, as it is something that does not seem bad enough for people to really think about, but it can be very hurtful. The origin lies in the scale of the association, which is a pitfall within itself but can also be a strength when people try to be there for each other and support each other.

Do you have any last comments?

Siza is leaving in January and will therefore be leaving her tasks as a confidential adviser as well. If there is anyone who is interested in becoming a confidential adviser for the ACD, please contact the board at bestuur@acdweb.nl. If you have anything you wish to talk about in confidence you can contact vetrouwen@acdweb.nl. Take care!



Anabolic French Toast

by Jiri Sanramat

Admit it, during this winter break both you and I had a bit of turkey; maybe also a bit of the Christmas cake, a few glasses of Glühwein, some mashed potato, and a couple of those nice cookies that your aunt made as her only contribution to the diner. After all of this Christmas goodness, you either gained a ton of weight, or you are one of those lucky few that has a metabolism faster than Kylian Mbappé (couldn't be me). So as a New Years resolution you have decided to go to the gym, and train those pounds off. You may quit after two times, or you've become a gym rat and can't even enjoy a cappuccino due to all the calories it contains (80 kcal). For the latter ones, I have the perfect breakfast recipe for you: Anabolic French Toast (wentelteeftjes) - inspired by Coach Greg¹ and perfected by yours truly. Of course, you can just make plain French toast by simply replacing all the sugar free ingredients with normal ingredients!

Ingredients (for 4 slices)

- 4 slices of white plain bread
- 2 egg whites (if you don't want this 'low calorie crap', take 1 whole egg and add 200 mL of milk instead of the two egg whites.)
- Cinnamon (to taste)
- Stevia/artificial sweetener (or sugar if you don't care about calories)
- Vanilla extract (to taste)
- Butter or margarine (really shredded people don't eat butter)
- Syrup or sugar free syrup

Preparation:

Add the egg whites to a bowl. Also add the cinnamon, stevia and vanilla extract to the bowl. Whisk until you have somewhat of a homogeneous mixture (you

will most likely not because the cinnamon is very hydrophobic and hard to dissolve).

Place a pan on your furnace and heat it, make sure that it is hot enough. Now add the butter or margarine and melt it. Take the bread and soak it in the liquid, until the bread has absorbed enough liquid that it becomes very soft. Don't soak it too long as your bread will become too soft which is difficult to grab!

Now bake your French toast in the pan until they're nice and golden. If you have liquid left, pour it on the bread while it is in the pan to absorb some extra protein (bro). After baking, serve the toast with a bit of syrup (or powdered sugar) and be ready to grow some muscles!

¹: <https://www.youtube.com/watch?v=z-p84S56h3U>



Interview with Jens Tolboom

What is it like to do a PhD?

Siebe Lekanne Deprez & Anna May Inzenhofer

As nothing lasts eternally, MSc. students eventually must choose between leaving academia or continuing in it. The choice can be quite difficult, so we (Anna May and I) decided to interview Jens Tolboom, a PhD candidate that started recently, to gain insights that may help current MSc. students with their choice.

Jens Tolboom started his PhD project in October 2022, as the follow-up of his BSc. and MSc. chemistry at the UvA/VU between 2017 and 2022. During his time as a student, he became increasingly interested in catalysis and synthesis. With his interests, it was clearly meant to be that he started working in the HomKat group on developing catalysts for accelerating the drying process of alkyd paintings. Yet, Jens argues that quite the opposite of “predestined” applies; he actually had some doubts about proceeding with a PhD and did not know for a long time what direction he wanted to take.



Doubts about doing a PhD and the motivation for choosing it

These doubts were about pursuing a career in academia or industry. Jens' most important consideration was to have room for his own ideas and personal development. During his time as a student, he realized that both academia and industry provide the space for this. However, he felt like the opportunity to gain fundamental knowledge is greater in academia. Moreover, the fundamental knowledge you gain in academia can also give you additional opportunities in industry.

In the end, two considerations convinced him to start a PhD. The first one is his belief in the project. In a conversation with Bas de Bruin, Jens became excited about a specific research topic and saw much potential for the idea to work. It led to the motivation to realize the idea. In addition, he felt (and still feels) very honored to have gained the opportunity to work on the project. The second consideration is about the HomKat group. Jens enjoys the group atmosphere and the feeling he gets from working within the group. Although doing a PhD is mostly individual work, he likes the challenge of becoming an expert on one specific topic. Also, his supervisors Bas de Bruin and Hong Zhang (photonics) motivate him, despite it not always being easy to work interdisciplinary.

Doing a PhD: daily activities and challenges

Now that Jens has practiced being a PhD for several months, he is willing to share his current activities and challenges. His daily routine is

the following: Jens wakes up at 6.40pm, takes a shower, eats breakfast and thereafter travels for one hour by bus and train to Science Park. He arrives usually between 8.00 and 8.10 am and the first thing he does is cleaning his workspace from the day before. So far, his schedule is fixed. But after cleaning, he plans out what he will work on that day: which reactions will he initiate today? Which compounds will he purify? What will he analyze?

Making these choices is one of the biggest challenges he faces. According to Jens: "Starting a project is easy; the most difficult part lies in continuing with a project and persevering." More often than not, he gets results that differ from his expectations and do not yield the desired product. He says that these setbacks can reduce motivation, but coping with them is important. Jens' way is to just accept that a PhD will always include difficult times. But, you should actually try to get comfortable with this discomfort: "So start something with the end in mind, and when you know what it takes to get to the end, then the whole difficult part in the middle will be less tough."

Moreover, Jens exemplifies a major practical challenge by mentioning a crucial difference between being a student and PhD candidate. As a student, it is possible to gain excellent exam results by memorizing reaction schemes by heart. Yet, as a PhD candidate, the challenge is to put theory into practice and make your ideas work. He already experienced instances in which he thought that a certain reaction would lead to a certain outcome, but produced different results instead. Facing this challenge, Jens advises to have trust in yourself and try different possibilities to make a reaction work, like trying a variety of conditions, reactants, etc. He reassures us that "most of the time, scientific literature really works."

Current research topic

But what is Jens' research actually about? His research topic is the drying process of paints, particularly alkyd paints. Paints of this type usually dry via autoxidation, which means that the resins in the paint react with oxygen when exposed to air. Autoxidation proceeds via a radical mechanism and contains the standard steps: initiation, propagation, and termination. The result is a large, crosslinked network of resins, or in other words, dry paint.



Polymer chains before (left) and after (right) chemical drying, with crosslinks in red.

So far, the catalyst developed by the group is only activated when exposed to air and blue light. Jens will continue this research and wants to develop a catalyst that increases the speed of paint drying and has other modes of activation. At the same time, he tries to become an expert in most of the analytical and synthetic tools required for his research.

Advice for chemistry students

Finally, Jens has some advice for chemistry students (both bachelor's and master's): you are the only one that gives you a direction for the future. "If you feel lost at this age, it is not really a problem, but you need to give yourself direction or a goal. It really does not matter how long you take to reach this goal. The path is more important than the speed of the steps you take. Take your time to figure out what you want to do, and to try to achieve your goal."



Sustainable computational chemistry

More than ones and zeros

Siebe Lekanne Deprez

Supercomputers have become indispensable in chemistry, but the current energy scarcity has made the energy consumption of supercomputers a major issue. Various measures are being taken to consume less energy, but the question is whether they are enough.

It looks futuristic: a sterile, white room with rectangular black cabinets the size of a human being. Thousands of wires run inside these cabinets to connect devices, and a deafening sound is created by the fans in the ground that requires the use of hearing protection. In front of your eyes is the supercomputer Snellius operated by Surf—the Dutch ICT cooperative. Snellius is the most recent and largest supercomputer in the Netherlands and several scientific fields are using it to perform calculations that are too demanding for normal computers. For example, chemistry occupies a substantial portion (30%) of Snellius' computing capacity.

But, Snellius has a dilemma, as its energy needs have to decrease due to economic developments and an increase is required for current expansion plans. The war in Ukraine has created energy shortages and energy prices have risen significantly. According to the sustainability advisor of Surf, a significant portion of their budget goes to energy costs, and those costs have certainly doubled last year. Surf is now even considering setting an energy limit. This may affect the computational chemistry sector and cast doubt on plans to expand Snellius to compete internationally. Therefore, it is now relevant to examine what measures Snellius is taking to

become more sustainable, and what impact this will have on computational chemistry.

First, it is important to consider why computational chemistry needs Snellius. Today, computational chemistry requires supercomputers to make new findings. The more powerful the supercomputer, the more reliable the results, but also the more energy is required. Using simulations of molecules, researchers can help solve societal problems, such as developing person-centred cancer drugs and making more efficient solar panels. But, the downside of supercomputers is that all that computing power requires a lot of energy, much of which is lost in the form of waste heat.

Yet Snellius' current energy needs are not too bad compared to foreign supercomputers and it is even one of the most sustainable supercomputers in the world. Yearly, Snellius consumes as much energy as two thousand households while other supercomputers use around ten thousand for the same amount of computing power. The major difference is the result of Snellius being designed to be as sustainable as possible. Globally, Snellius ranks 439 in terms of computing power, but 13 in terms of energy efficiency (the amount of energy needed to perform a calculation, ed). Being sensible about sustainability is also important because the Netherlands simply has few renewable resources; the Netherlands is small and flat and obtains renewable energy mainly from wind power. France, on the other hand, has more options such as nuclear power and hydroelectric power.

So how exactly does Snellius take sustainability into account? By using specific hardware (equipment) and optimising algorithms. Traditionally, the same hardware was used to perform all kinds of calculations, but today's hardware is being developed to perform one kind of calculation extremely efficiently, resulting in less energy consumption. Surf's advisor relates the development to our use of cars: "Everyone used to drive the same car in the early days, but now you have trucks, passenger cars, buses, etc., each with a specific purpose." Moreover, Snellius pays very close attention to whether the algorithms are optimized. This means devising algorithms make the calculations less demanding to execute, resulting in less energy consumption.

In addition, Snellius also considers reusing residual energy. Performing calculations creates a lot of heat. Powerful fans are needed to dissipate that heat; if the temperature rises too much, the supercomputer will malfunction or even melt. Snellius uses a cooling system in which hot air from the supercomputer transfers heat to water in a room next to the supercomputer. The water heats up and is then used to heat neighbouring buildings. This process makes Snellius' cooling system circular and sustainable.

From a computational chemist's perspective, there is another, indirect way of preservation—saving resources that do not need to be used. For example, when a drug is developed, often thousands of trials are undertaken to identify potential drugs. Hopefully, one will obtain a suitable candidate. By using the computer, the screening process is greatly accelerated without wasting raw materials and chemicals. But, the question is whether this does not displace the problem since supercomputers contain components made up of scarce materials such as lithium. Often, the parts have to be replaced after only a few years and this does not benefit sustainability. So, it is important to put resource savings in perspective with the supercomputer's

required components.

Despite these measures to reduce energy requirements, the question is whether they are enough given the planned expansions of Snellius. In the coming years, Surf plans to expand the supercomputer twice to meet the increasing demand for computing power. One of the reasons why the expansions are needed is because other disciplines now want to use supercomputers as well. According to Surf's advisor: "Supercomputers are mainly used by beta sciences with physics and chemistry as the main stakeholders, but we are now also seeing IT and financial companies wanting to use Snellius to perform data analysis." This causes Surf to have to choose who gets to use Snellius, as there is more demand than supply. But right now, it is unclear how Snellius' expansion plans will be affected by the energy scarcity.

In short, energy scarcity makes sustainability a crucial topic for Snellius. Despite the fact that Snellius is one of the most sustainable supercomputers in the world, it is in a tough spot. There are opposing desires including plans to expand Snellius as well as the need to reduce energy requirements. Since there is a close collaboration between computational chemistry and Snellius, the energy shortage may result in a larger competition for chemistry to be able to use the supercomputer. Computational chemistry research may be delayed as a result. So computational chemistry is not only about ones and zeros, but also about the factors that influence how those ones and zeros come about.

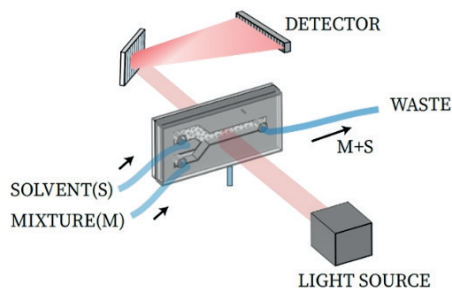
Disclaimer: This article was written for the course "Science Journalism" (part of the Major Science Communication). The target medium is the C2W magazine and thus the target audience is chemists in the broad sense. The article is written in a pop-science style which differs quite a lot from writing in an academic style. Maybe you can guess the differences?

InfraRed Diffusion Ordered Spectroscopy

Anna May Inzenhofer & Rianne van Diest

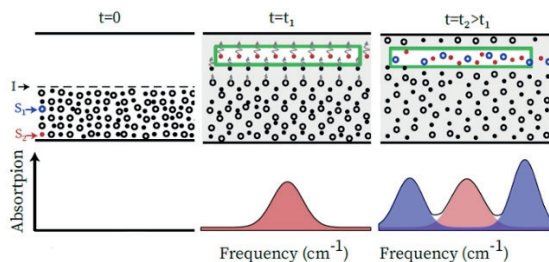
You might have seen it in the HIMS-news already: prof. dr. Sander Woutersen and dr. Giulia Giubertoni have developed a new chemical probe, called infrared-diffusion-ordered-spectroscopy (IR-DOSY). This new technique enables the simultaneous analysis of molecular size and structure. They already received a Demonstrator Grant from the Dutch Research Council NWO to develop IR-DOSY further for analysis or diagnostics, in collaboration with the Demonstrator Lab Science Park, and this fall, a paper about the new technique was accepted in *Angewandte Chemie*.¹ Two students have been working on this project as well: Gijs Rombouts has helped with the development of IR-DOSY, and Rianne van Diest has been looking into the application of IR-DOSY for the analysis of protein aggregates. We thought this might be a nice opportunity to update everyone about this new analytical technique and its potential applications!

Gijs, now a master's student, contributed to this photonics project for his Bachelor's project. He agreed to share with us a bit about what such a project entails. So, let's get right into it. The IR-DOSY setup consists of a y-shaped spacer cell, with calcium fluoride windows on both sides, and a metal plate with a slit in front of the cell. As we see in Figure 1, two flows enter the y-shaped cell, the bottom one being a mixture of compounds with a different size, and the top one being the solvent. When both solutions have a similar viscosity and are injected with the same flow speed, there will be an interface in the middle of the channel.



▼ Figure 1: The setup of the IR-DOSY cell. The y-shaped spacer has two inlets for the solvent and mixture respectively. A metal plate with a slit (not shown) directs the IR-beam to the top of the channel.

As Gijs explains, “At the top of the channel, a slit allows an infrared laser to shine through. As long as the flow is steady, you will only measure the solvent, because the IR-beam does not extend across the interface. However, when the flow through the cell is stopped (at t_0), Brownian motions cause the molecules of the mixture to diffuse across the interface into the IR light, so that their IR-spectrum can be measured.” From the Stokes-Einstein equation, $D_{SE} = k_B T / 6\pi\eta r$, we can see that the diffusion coefficient is inversely related to the radius of a particle. This means that the smaller molecules will diffuse faster across the channel of the cell. As a result, the smaller molecules will be the first to move into the IR-beam, while the larger molecules will follow later. This time dependence allows the IR signals to be temporally separated by their molecular size, and based on the diffusion time, their respective diffusion coefficients can be derived. By subtracting the IR-spectrum of the smaller molecules from the spectrum of the larger molecules, the IR-spectra of the compounds in the mixture can be disentangled. An example is shown in Figure 2.



► Figure 2: IR-DOSY measurement. At $t=0$, all molecules from the mixture are in the bottom part of the channel, and the solvent is in the upper part. After time $t=t_1$, the smaller molecules (red) have diffused across the channel into the IR-beam (visualized with a green rectangle) and their IR-spectrum can be measured. After another time $t=t_2 > t_1$, the larger molecules (blue) have diffused this distance as well, and now the IR-spectrum of both molecules will be measured simultaneously.

Why IR-DOSY and not NMR-DOSY? Well as we chemists like to say, it's another tool in the toolbox. NMR-DOSY has its advantages, but it is not so suitable for the elucidation of complex supramolecular compounds, like protein aggregates or some molecular cages. Assuming the compounds can be dissolved, IR-DOSY could potentially provide clearer images. And in this age of microplastics, too big for NMR and too small for microscope images, IR-DOSY could provide a clearer way to understand their reactivities.

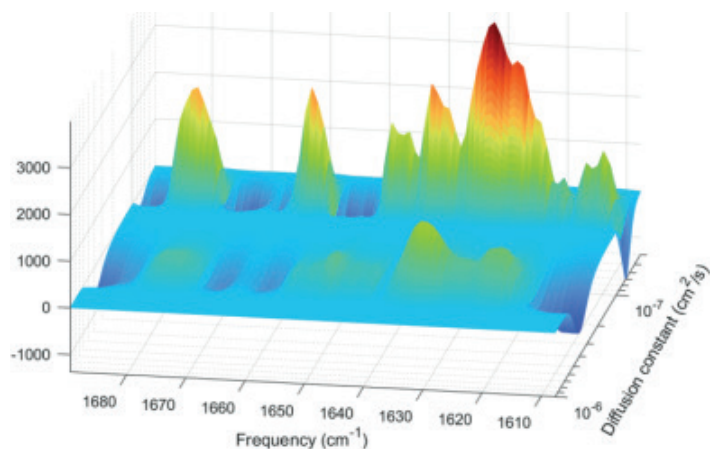
A large portion of Gijs' project had to do with fundamental engineering aspects, which were done in collaboration with the physics department. For instance, a laminar flow through the cell, as opposed to a chaotic, turbulent flow was required for a stable interface. The interface could be adjusted based on the flow speed and viscosity of the liquids. A stable interface between the two flow streams was required for an accurate determination of the diffusion coefficient. Towards the end of his project, a goal was a proof-of-concept measurement of nano plastics. For this, Gijs dissolved PET with TFA and encapsulated it into SDS micelles.

I asked Gijs what his favorite part of the project was, to which he replied, "being included in the discussions and brainstorming sessions with my supervisor about the project." A not so nice part, however, was the method he used to break down PET which was to literally grate a PET bottle with a cheese grater. The literature procedure he

used required 2 grams of PET shavings for each reaction. If the follow-up encapsulation reaction did not work, he would grate another 2 grams of PET.

What does the future of IR-DOSY look like? Well, the current set-up has some hurdles to overcome. As the diffusion time (and thus the measurement time) directly correlates to the molecular weight, measuring large molecules is time-intensive. This was exactly the problem Rianne encountered in her project, where she studied amyloids with IR-DOSY. Amyloids are a specific type of protein aggregates that can be found as plaques in the brain in Alzheimer's and Parkinson's disease. They are characterized by β -sheets, but their IR-spectrum can be difficult to disentangle from monomer proteins, especially when the monomer already contains β -sheets. With the set-up as discussed above, measurements would take up multiple days, or even no diffusion of aggregates could be measured at all, probably due to gravity hindering the diffusion upwards in the channel.

To solve this problem, the set-up of the cell was switched around: instead of placing the slit at the top of the channel, it would be placed at the bottom of the channel, at the site of the mixture. Now, instead of waiting for the molecules to arrive into the slit area, you can monitor the depletion of the smaller species. The IR-peaks belonging to the small molecules will be reduced by 50% in intensity, while the intensity of the peaks belonging to the larger molecules will be



► Figure 3: IR-DOSY spectrum of a mixture of beta-lactoglobulin monomers (front) and aggregates (back).

consistent. For Rianne's project, this method (depletion IR-DOSY) allowed disentangling the similar IR-spectra of protein monomers and aggregates separately, as shown in Figure 3. A drawback is that the diffusion coefficient, and therefore the size of the non-diffusing aggregates cannot be determined. However, in Parkinson's or

Alzheimer's disease, monomers, smaller protein aggregates, and amyloids will all be present at the same time in the body, which makes depletion IR-DOSY an interesting tool for diagnostics. But first, the demonstrator grant will be used to further optimize the IR-DOSY technique and make it fool-proof, so that everyone can use it.

I. Giubertoni, G.; Rombouts, G.; Caporaletti, F.; Deblais, A.; van Diest, R.; Reek, J. N. H., Bonn, D.; Woutersen, S. *Angew. Chem. Int. Ed.* **2023**, *62*, e202213424.

Chemistry vs. Political Science

Anne-Fay de Jong

Political Science

First of all, what is your name and why do/did you study Political Science?

N: Hi, I am Noa Bakker! I decided to study Political Science (PoliSci) since it provided a nice combination of analyzing history, societal problems and international relations; all things that fascinate me a great deal.

L: My name is Laura Austin and I studied PoliSci because I was curious about the world and how the world works. For me PoliSci entails a scientific approach to the structures, such as our society, that make up our world and our experiences of it.

What do you think Chemistry entails?

N: I have to admit that I do not have a detailed idea of what it entails, but I'd imagine that the study is focused on analyzing and studying chemical processes and reactions, and how they influence one another.

L: I think Chemistry has many definitions. Chemistry, as a study program, I think entails learning about the structures of our physical world. It is an exact science to explain the physical phenomena that we encounter every day, involving a lot of calculations to make sense of these phenomena.

Who is 'the' Chemistry student?

N: I would argue that 'the' typical Chemistry student is a person who reasons from facts rather than morals, proceeds in a precise manner, is intrigued by what goes on on the micro-level, and is therefore very interested in the nitty-gritty of the subject they are studying.

L: I feel like 'the' Chemistry student is a student with an intrinsic motivation to explain things, such as the daily phenomena I just mentioned. I might be wrong but I think 'the' Chemistry student is someone who wants to explain and improve. On a stereotypical note, I feel they have to have a certain affinity with numbers and the nitty-gritty of the things they're trying to explain.

How do Chemistry students overestimate themselves?

N: I think a Chemistry student can overestimate the power of their argument by claiming that their knowledge is objective because it is supported by 'actual' research. During my studies, I was constantly encouraged to be critical about whether a concept like objectivity even exists. I can imagine that a chemistry student could possibly ignore their own bias and influence on the subject being studied.

L: Probably, by thinking that every single natural phenomenon or layer of the natural world can and should be explained. With this I mean, that the exact sciences do not leave much room for philosophical/social considerations because they don't prioritize them. I believe that there will always be natural phenomena that cannot and maybe should not be understood or explained and chemistry students probably overestimate the scope of human understanding in that way.

In what do Political Science students overestimate themselves?

N: I would say that PoliSci students overestimate their ability to 'win' an argument or sound convincing solely because they tend to be good at putting things into words. Being good at arguing does not necessarily mean that the person in question always knows best; they simply know how to sound convincing.

L: In my opinion, most PoliSci students want to change something. Whether it's a political institution or societal injustice, they usually have a very expansive goal. I think PoliSci students overestimate themselves in that they believe that they might actually achieve said goals and 'change the world'. It is a little idealistic and maybe slightly narcissistic. However, I do hope that most PoliSci students keep a little bit of this overestimation and do not get completely crushed by the system and keep trying!

What are Political Science students better at than Chemistry students?

N: Most of my fellow students were very capable of articulating their arguments in a very detailed manner and that usually led to interesting arguments and discussions. I think Chemistry students might struggle to do this as efficiently.

L: I want to say 'seeing things from different perspectives', because I believe chemists do not prioritize the philosophical/social considerations of certain issues, while PoliSci students are taught to do just that. I feel like in Chemistry, as an exact science, there are less nuances in all considerations made. Chemistry students are taught certain approaches, like math equations etc, to solve problems, and perhaps those considerations are less present because that would make Chemistry more abstract and not perceived as "truth", which PoliSci almost has nothing of. As a PoliSci graduate I feel that every institution and societal issue has its own truth that changes on the basis of who's looking at them.

What are Chemistry students better at?

N: I would imagine Chemistry students being better at doing a deep dive into a specific topic and not letting go until they have found a definitive answer (if that even exists). In PoliSci, a lot of articles or research papers end with the conclusion that 'further research is encouraged'. I think it's good to acknowledge the limits of one's own research, but it sometimes comes across as an easy way out to an actual answer. However, I do think that it also depends on the topic in question; chemistry might allow more definite answers, while questions about societies or political struggles are ever-evolving.

L: Math. But seriously they probably are. Moreover, I think Chemistry students are better at making decisions. PoliSci can get so abstract and subjective sometimes that it's difficult to have a useful/productive discussion, whereas Chemistry students are probably better at looking at the facts, discussing those, and then making a decision based on the said process.

What do you think is the major difference and the major similarity between Chemistry and Political Science students?

N: The major difference is the way in which research is approached; as I mentioned earlier, I can imagine that a Chemistry student is looking for a definitive answer, while PoliSci students do not approach their study with this idea. A similarity between the two studies is combining knowledge to get a new result or a better understanding.

L: I think the major similarity is the need for knowledge on "how the world works". Both Chemistry students and PoliSci students want to understand structures and processes. I think then the major difference would be the topics which they would want to understand. Also, Chemistry students might want to explain more and PoliSci students want to understand more.

What do Chemists do all day?

N: I suppose that they spend a lot of time in laboratories, studying chemical reactions and processes.

L: Worry about their titration finals maybe? No, just kidding a little high school flashback. Probably constantly trying to improve existing explanations, processes and approaches while simultaneously trying to find new ones for other problems and phenomena they might not even know exist yet. That is the beauty of the exact sciences: we know so much and yet almost nothing.

Chemistry

First of all, what is your name and why do you study Chemistry?

O: My name is Ole van Tiel, I am a second-year bachelor's student, and I study Chemistry because I think it's cool how the world is built up on the atomic scale. I also like how chemistry can be combined with physics.

B: I am Bibi van Poelgeest and I currently study Chemistry (Analytical track). I have chosen this master's as I am passionate about science, especially chemistry. I enjoy the possibilities and opportunities chemistry provides, as it is part of everything you could think of.

What do you think Political Science entails?

O: I think PoliSci is about the problems our

modern world faces, like overpopulation and terrorism, and how they might be solved.

B: I have no clue what to expect in detail, but I think PoliSci takes a closer look at both political choices and occurring political problems on a small (regional) and big (worldwide) scale.

Who is 'the' Political Science student?

O: The PoliSci student is someone who cares about others and the world around them. They want to solve the problems to make the world a better place for the next generation and like to debate with people about all kinds of politics-related topics.

B: I have never met one, but my assumption would be that a PoliSci student would be a very social person; interested in political problems and how these can be solved. I think they are way more aware of behavior and politics than most Chemistry students.

How do Political Science students overestimate themselves?

O: They think they know everything about the political system, which makes them think you are wrong, even though you might not be.

B: If I had to guess, PoliSci students are more into Social Sciences than Natural Sciences. Despite their background, politicians do have to tackle problems related to Natural Sciences. They could underestimate the chemistry behind a problem and overestimate their knowledge of the problem and make an inappropriate decision.

In what do Chemistry students overestimate themselves?

O: Chemists often think they are better than other students, especially humanities students.

B: I think Chemistry students often overestimate themselves by thinking that the world is underneath their feet, just because they have done a Natural Science study. They belittle Social Sciences, which is unfair.

What are Chemistry students better at than Political Science students?

O: Practical skills, not just in the lab but generally.

B: I think Chemistry students are better at reviewing the 'iceberg' behind natural science-related challenges. They should be capable of

looking a step further and looking for the possible answer to a problem, such as what makes the answer true and what are its limitations.

What are Political Science students better at?

O: Human knowledge.

B: PoliSci students should be better at the social events occurring with political challenges. I think they can combine behavior and patterns to obtain a solution to a political challenge and have a better idea of how people would respond to a decision.

What do you think is the major difference and the major similarity between PoliSci and Chemistry students?

O: Both types of students think about how the world works and are trying to find ways to make the world a better place. They differ in how they look at the world, chemists think of atoms and molecules, whereas PoliSci students think of people and politics.

B: The major difference is in the way both students view a certain problem. PoliSci students would take a closer look at the social side of the problem, while Chemistry students would think about the chemistry behind the problem. For instance, when taking a closer look at plastic a PoliSci student could take a look at how we can change the usage of plastic (less single-use products), while chemists could create an alternative for plastic (a new bio-based and biodegradable plastic).

The major similarity is the analytical mindset. I think students from both studies should be capable of analyzing the structure and/or patterns behind a problem. Even though they will look from different angles, both opinions are necessary to solve a political challenge.

What do Political Scientists do all day?

O: Debate about everything.

B: I think they have, similar to chemists, many different job opportunities. My guess would be that they are often found in politics-related jobs, or something in consultancy, where they study behavior and political patterns to find a solution or give advice for a problem.



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Smaakmatrix

Inspired by the Parool

Scientific

● People are becoming less hot (in body temperature)

● Sperm count in males has gone down

● James Webb telescope is performing better than expected



● The blad is looking for members!

● Fireworks are back, and so were all the accidents

● Winter-wonder Ball

● Megan from temptation island is being accused of fraud

Horrible

Beer-related