

From the Frontiers of Knowledge  
Cutting-Edge Science in Groningen - p. 8 - 26

Proton Therapy Planning  
KVI-CART - p. 17 - 19

# Periodiek

Recurring Magazine | Issue 2018-1

Astrochemistry: the First Step in  
Understanding our Origins

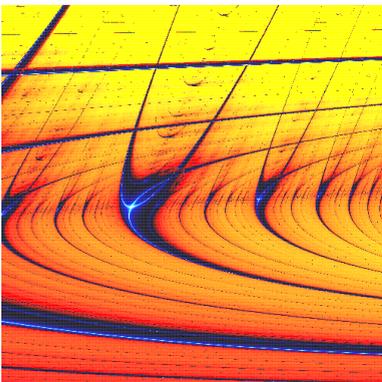
Veronica Allen - p. 8

*FMF*

---

## 8 - Astrochemistry: the First Step in Understanding our Origins

On behalf of the Kapteyn institute, Veronica Allen tells us about chemistry in molecular clouds. Understanding the chemical processes involved in producing organic molecules in space will lead to a better understanding of how life itself begins.



## 20 - Exploring Complex Dynamics with Lyapunov Exponents

Dr. Alef Sterk from the Johan Bernoulli Institute tells us about dynamical systems. We will consider a model from mathematical biology which describes the population size of successive generations of a certain species. We will explore the behaviour of a dynamical system which can become chaotic in some specific cases.

## 27 - Vinyl Records: The Road from Studio to Loudspeakers

FMF members Rick van Voorbergen and Robert van der Meer talk about vinyl records. How are these black disks — that are nowadays again very popular — made, how does a record player read off a signal from small grooves and how is this signal eventually strong enough to drive a loudspeaker?



- 4 In the News
- 6 From the Board
- 8 Astrochemistry:  
The First Step in Understanding our Origins
- 14 Theory in Support of Experiments on Atoms and Molecules.
- 17 Advanced CT Imaging for Accurate Proton Therapy Planning
- 20 Exploring Complex Dynamics with Lyapunov Exponents
- 24 Jumping in the Solid Phase:  
Perovskites for Solar Cells and Beyond
- 27 Vinyl Records:  
The Road from Studio to Loudspeakers
- 30 Brainwork: Count Count
- 31 Recipe: Cream Puffs

## From the Editor in Chief

It is a pleasure to present to you the new edition of the Periodiek. It is pimped with an orange theme, which would probably not be the case if we hadn't welcomed a reinforcement to the board of editors, being Josselin.

As usual, this magazine is packed with interesting articles, puzzles and other stuff. For example, if you have always wondered how we play music with a phonograph record then you can read the article written by two FMF members.

As I figured out myself the hard way, the puzzle is quite a challenge this time. So to warm up your brain you can start by figuring out why this month (February) has 8! minutes.

-Gerrit van Tilburg

### Editors

Jonah Stalknecht,  
Gerrit van Tilburg,  
Jasper Somsen,  
Josselin Kooij,  
Rick Vinke

### Authors

Marc-Jan van Goethem,  
Joanne K. van Abbema,  
Emiel R. van der Graaf,  
Anastasia Borschevsky,  
Rick van Voorbergen,  
Robert van der Meer,  
Sytze Brandenburg,  
Thomas Jansen,  
Jasper Somsen,  
Veronica Allen,  
Rick Vinke,  
Alef Sterk

### Advertisers

KxA (p.13),  
ASML (p.23),  
Schut(p.32)

Advertise? Contact us at  
bestuur@fmf.nl.

**Print run** 1100 pieces

**Press** PostNL

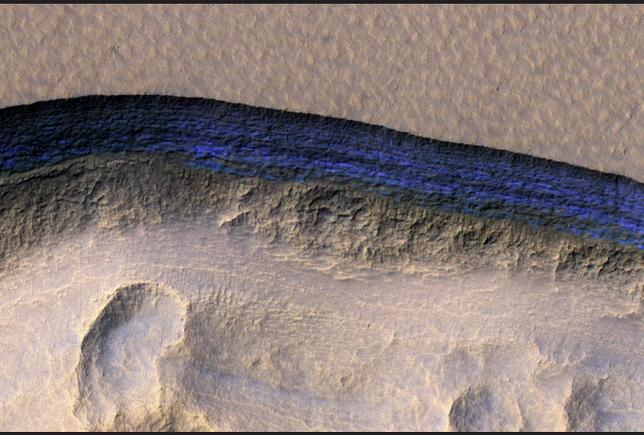
**ISSN** 1875-4546

### The Periodiek

is a magazine from the Fysisch-Mathematische Faculteitsvereniging and appears four times per year. Previous issues can be found at [perio.fmf.nl](http://perio.fmf.nl). The board of editors can be reached at [perio@fmf.nl](mailto:perio@fmf.nl).

The logo for FMF (Fysisch-Mathematische Faculteitsvereniging) is displayed in a stylized, italicized font.

# In the News



Wired



Scientific American

## Clean water ice just below Mars' surface

It has been known for a while that at certain locations, there resides some amount of ice below Mars' surface. But the specifics of this ice have long been a mystery to planetary geologists. The cleanness and amount of the ice is very important for possible manned missions to Mars in the future.

Erosion on the surface of Mars has allowed scientists to peek a glance at the ice directly. In a recent article in *Science*, Dundas et al. published their observations: they found an ice layer with a thickness of 100 meters or more. It is expected that this layer preserved a record of Mars' previous climate, which makes it interesting for future research.

This ice layer is very close to the surface, at some locations only at about 1 or 2 meters depth. This makes the ice very mineable, which is expected to make it a useful source of water for future human missions on Mars.

SCIENCE

## Self-healing concrete using fungi

Cracks in concrete can be very dangerous, as they lead to damaged bridges and dangerous roads. The smallest of cracks progress and grow over time and will eventually require costly repairs.

Assistant professor Congrui Jin from Binghamton University recently published a paper in which he proposes a possible solution for the crumbling infrastructure: self-healing concrete that would fix the concrete permanently. Jin and her team found a solution using a fungus called *Trichoderma Reesei*.

Fungal spores are placed in the concrete, and when the first cracks in the concrete appear, the dormant fungal spores will grow and produce calcium carbonate which heals the cracks.

When the cracks are completely filled, the fungi will produce more spores. These spores could be awakened again when more cracks form, and the process starts over.

BINGHAMTON

## New metalens focuses all visible wavelengths to the same point

A metalens is a flat surface that utilises nanostructures to focus light. A team of researchers at Harvard John A. Paulson School of Engineering and Applied Sciences (SEAS) have for the first time developed a metalens that focuses every wavelength of light in the visible spectrum to the same point.

Every different wavelength of light moves through a material at a different speed, which makes the focusing of every colour of light to the same point a difficult task.

Optical devices such as cameras correct for this difficulty by using multiple lenses with different curvatures and thicknesses, which adds a lot of bulk to the device. Here these new metalenses have a big advantage over traditional lenses.

The next step is to scale up the metalens. This could lead to interesting applications in new devices such as virtual and augmented reality.

SEAS HARVARD

## Problems with CRISPR in humans

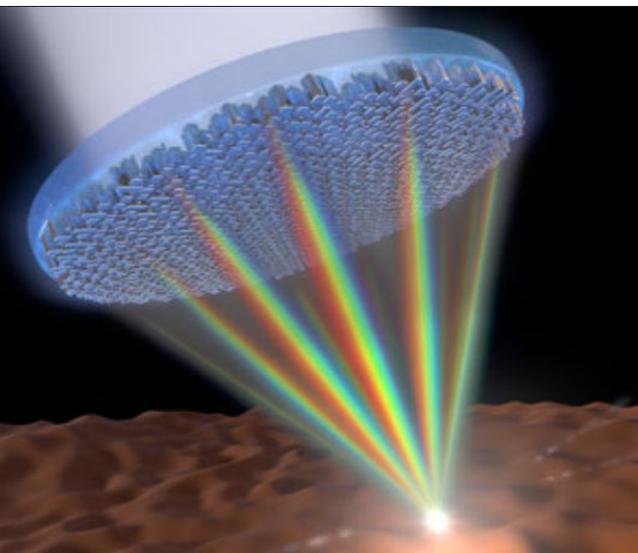
CRISPR is a relatively new and promising tool for DNA editing. In 2013 human cells have been edited for the first time, the possibilities are thought to be near endless.

CRISPR in humans is supposed to take a great step in 2018, with the first clinical trials in the US and Europe to treat diseases.

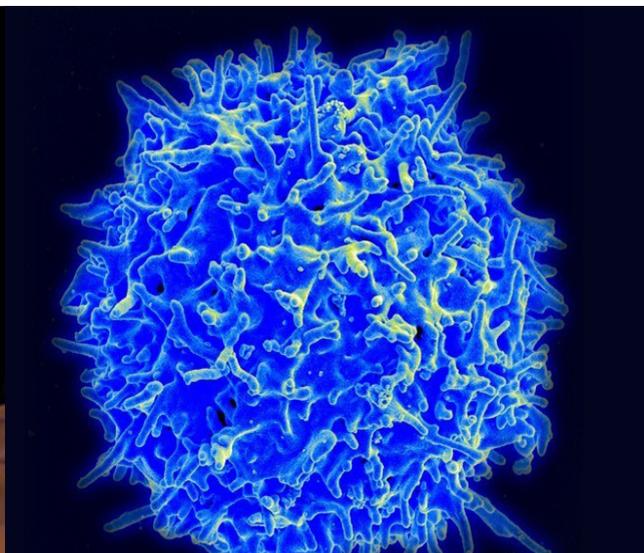
However, 2018 started off differently. A new (not yet peer reviewed) paper suggests that many humans may already be immune to CRISPR. CRISPR comes from bacteria that many humans may have built up an immunity for. 65% of people are found to have antibodies that react with Cas9.

But this is not the end for CRISPR in humans: Cas9 can still be used outside the body, or at other places the immune system cannot reach. Also, Cas9 can be modified to use a different CRISPR protein altogether.

THE ATLANTIC



SEAS Harvard



The Atlantic

---

# From the Board

## Commissioner of Educational Affairs

AUTHOR: RICK VINKE

A few years ago, in the academic year 2014-2015, the board gained a sixth function, then called the Commissioner of Education. Its purpose? To take up “any education-related tasks, besides the usual board tasks [1]”. That may sound very vague, and that’s because it is vague. I’ll try to tell you what I do and how I ended up at this function, so you can think of your own definition.

### How did I get myself into this position?

My humble beginnings lay in a customer-oriented supermarket, where quality precedes price. This absolutely boring job as a stock boy gave me great insight in what I did not want to do when I grew up. While this is a nice way to get such insights, it is very time-consuming and slightly depressing.

I think that it’s very important for people to orient themselves on what they want in life, in particular the job they will potentially do half their lives. Most people do this by looking for the things they like in a job or a study, but I believe that it’s equally valuable to look for the things that you don’t like. As stated, being a stock boy for a long time is a way of discovering the detestable things in some jobs, but it could be easier. Another way is doing extracurricular activities next to your studies. Someone has to organise these activities, and that’s where the Commissioner of Educational Affairs plays a large role within the FME.

When I was in my second year of my Bachelor’s in Physics, after completing the propedeutic phase, I got a job as a teaching assistant. The fact that this paid three times as much per hour and was infinitely more fun than being a stock boy, meant that I left my job at the supermarket, the end of an era. At the end of my third year I had had six TA positions, and got my Bachelor’s degree. Not wanting to start my Master’s immediately, I applied for board of the FME, for the function Commissioner of Education.

### Why?

My motivation for applying came from the things mentioned above: I wanted to help people orient

themselves on future jobs, but also help them in their studies. This is largely achieved by collaborating with fellow board members, but also with the staff of the Faculty. The fact that the other applicants for board positions were already friends of mine makes part of this collaboration easy and fun. The other part, interaction with staff, was something I didn’t know much about when I applied, but it also turns out to be one of the better aspects of the position, mainly due to the fact that most staff members are very nice people to work with.

As of now, I still don’t regret applying for the function of the Commissioner of Education.

### Defining the Commissioner

According to the articles of the association, the Fysisch-Mathematische Faculteitsvereniging has the following aims, and realises them by:

#### Article 2

##### 1. The aims of the Association are:

- a. to help to broaden the academic training of its members
- b. to promote contact among students, and between students and academic staff
- c. to represent the interests of its members, insofar as the interests relate to their studies or future work environment.

##### 2. The Association attempts to realise these aims by:

- a. organising excursions and lectures
- b. working together with associations and institutions with a similar or related aim
- c. using all other legal means that could help to achieve these aims.

A fairly large part of the article represents what the Commissioner of Educational Affairs aims to do. The FMF organises a lot of extracurricular activities, and a large part of them is educational or helps job orientation. One wonders why my function wasn't created earlier. I hope that you now have some idea of what the function entails, as I'll go into some more detail in the next section.

### What I do all day

One of the first things I did when I became a board member, was changing the title of my function to 'Commissioner of Educational Affairs', mainly due to making it in line with the titles of the Commissioners of Internal and External Affairs. While such executive decisions take up a lot of time, this doesn't fill up a whole day. So what do I do all day?

Mainly, I keep in contact with the directors of the institutes to get, for example, articles for the *Periodiek*, as can be read in the 'From the Frontiers of Knowledge' section. Or to set up collaboration for another activity at the KVI-CART as was done in the past. When a Tuesday lecture is given by someone from the university, then that's probably also something I set up. All in all this is a small portion of the things I do daily.

Next to my board tasks, I'm also still a TA. It's a nice source of income, but also a way to spot flaws in certain courses. The usual way of improving them is by filling out the evaluation forms the Programme Committees

provide at the end of the course, but (assuming you passed the course) this only helps the people in the coming years. So when a course turns out to have some flaws, such as a professor that might not explain things the way you find useful, you have to turn to alternatives. That's where the study associations come in. Exam databases, practice sessions, Catch-up sessions: in a few years, you don't even need lectures and tutorials anymore to pass your courses.

The Catch-up sessions are a new concept I set up this year, where a teaching assistant gives a small lecture, recapping the material of the course, in order to get people who think they're failing back up to speed again. Organising these also take up a fair amount of my time in a period.

The course-related excursions, such as the one to Avantes with Waves & Optics, are also part of my function. Making these excursions happen require contact with the programme director, the company involved and the course coordinator.

All-in-all the Commissioner of Educational Affairs is a function that has grown a lot, and still has potential to grow, and I already look forward to what my successors will do to make it even greater than it already is•

### References

[1] Oudshoorn, M; Vinke, R.S.; Overdrachtsdocument Commissaris-Onderwijszaken der FMF, 2018



FIGURE 1: The most popular Catch-up session as of now: Linear Algebra 1, with a stunning 91 attendees!

## Astrochemistry: the First Step in Understanding our Origins

AUTHOR: VERONICA ALLEN

In any given molecular cloud – quiet, collapsing, or turbulent – chemistry practices its endless, slow dance: forming new molecules and dissociating others for eons throughout the history of the universe. These cold, dense clouds are the starting point of star formation and can be as massive as thousands of suns.



Stars form surrounded by disks of gas and dust where different molecules can be formed.

<https://photojournal.jpl.nasa.gov/catalog/pia03243>

Depending on a number of factors, including gas temperature and density, we find that chemistry has produced gas with considerably different compositions within these clouds. The interdisciplinary sciences of astrochemistry and astrobiology have experienced a surge of interest in recent years due, in part, to the detection of a multitude of extrasolar planets which could harbor life, and to the discovery of living things on every corner of Earth – from the deep oceans to extremely acidic or alkaline environments. Understanding the chemical processes involved in producing organic molecules in space, especially in star and planet forming regions where

these raw materials can be delivered to young planets, will lead to a better understanding of how life itself begins.

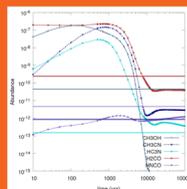
### Astrochemistry Triad

Astrochemistry is the study of reactions and interactions between atoms and molecules in space. In the field of astrochemistry, observers, theorists, and experimentalists are tightly bound to one another (Figure 1) and communication between the three groups is difficult but necessary. Experimentalists test the effects of different astronomical phenomena (like high energy radiation) on chemical reactions in

## Laboratory Spectroscopy



## Astrochemical Modeling



Molecules of interest  
Reaction and molecular parameters

Transition frequencies and strengths  
Unidentified lines

Abundance predictions  
Physical Conditions  
Molecular abundances



## Observational Astronomy

**FIGURE 1:** The three groups working in astrochemistry are deeply dependent on each other.

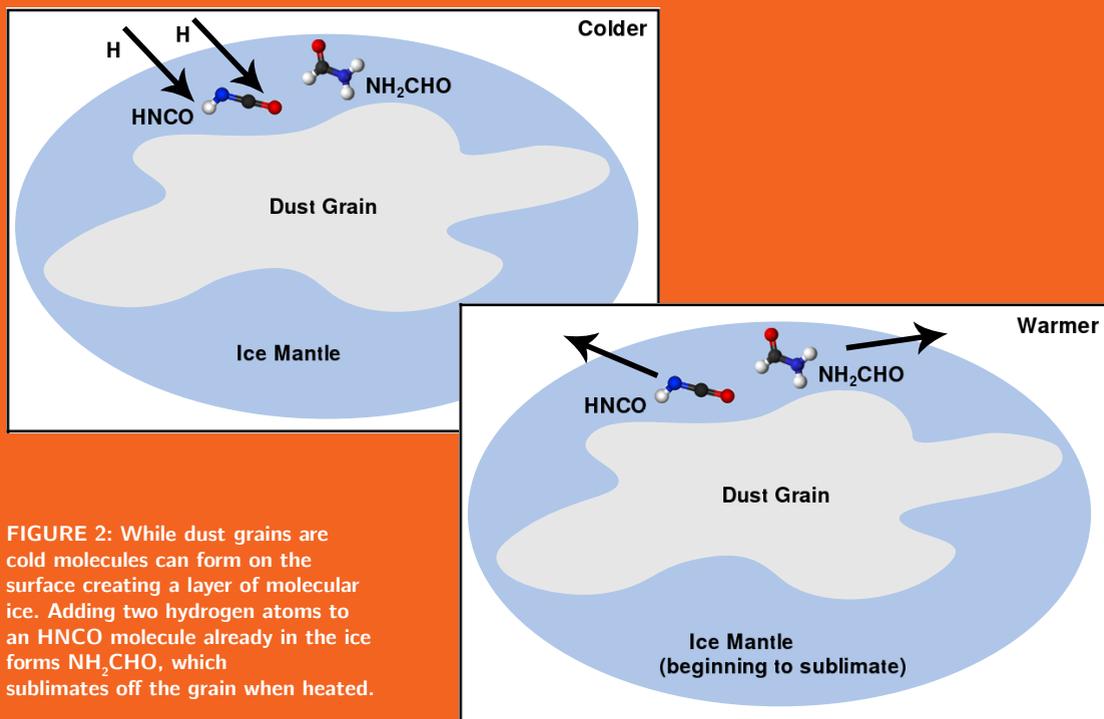
a vacuum (or as close to a vacuum as we can achieve on Earth). These results are used by theorists to create chemical models that can show how the abundances of different molecular species change with varying parameters (like gas temperature and density) and over time. Observers study data from different astronomical phenomena and rely on laboratory tested or theoretically calculated frequencies to determine which spectral lines arise from which species and determine the chemical composition of their object. Theorists and observers work together using models to understand how the observed sources got their chemical composition, which at the same time confirms that the models can reproduce reality.

Oftentimes, spectral lines for which there is no clear identity are observed, then it may be the case that the database is incomplete for some species and the experimentalists seek to discover which species may be associated with a particular transition using spectroscopy. Observational astrochemistry has experienced a boom in recent years with the advent of the Atacama Large (sub)Millimeter Array (ALMA),

an incredibly sensitive array of telescopes that have the ability to detect very weak signals from rare molecular species. This gives observers the ability to characterise astronomical environments better than before with more accuracy and potentially greater chemical complexity.

### Hot Molecular Cores

In the process of star formation, there is a chemically rich phase during which molecular species are released from the icy mantles covering dust grains that have been warmed by the protostar (a star which is still gathering mass from the surrounding molecular cloud and has not begun fusion). Alternatively, molecular species could form in the warm gas surrounding the protostar. In high-mass stars, this is called a hot molecular core and in low-mass stars a hot corino. It is during this stage that we observe complex organic molecules (COMs), molecules with at least 6 atoms containing both carbon and hydrogen [1]. The detection of these species marks an important age milestone for high-mass protostars as they are quickly (within a few thousands of years) destroyed by the



**FIGURE 2:** While dust grains are cold molecules can form on the surface creating a layer of molecular ice. Adding two hydrogen atoms to an HNCO molecule already in the ice forms NH<sub>2</sub>CHO, which sublimates off the grain when heated.

radiation from the star. It is expected that some of these COMs will remain in ice in the outer reaches of a star-forming region or freeze out within the mid-plane of a protoplanetary disk at a later stage of stellar evolution and end up in comets or other star system bodies. This ice is important in an astrobiological sense, given that the delivery of organic compounds to a primitive Earth is likely to have been important in the origin of life. Prebiotic oxygen-bearing COMs like dimethyl ether (CH<sub>3</sub>OCH<sub>3</sub>); glycolaldehyde (CH<sub>2</sub>OHCHO), the simplest sugar; and ethylene glycol [(CH<sub>2</sub>OH)<sub>2</sub>], more commonly known as antifreeze have been well studied [2][3], while their nitrogen-bearing counterparts have not.

*“Observational evidence for the dominant formation route of formamide is contradictory.”*

### Formamide as a path to life

Formamide (NH<sub>2</sub>CHO) is an important molecule to study in the fields of astrochemistry and astrobiology because its structure and content make it a likely precursor for glycine (NH<sub>2</sub>CH<sub>2</sub>COOH), the simplest amino acid, and an important building block in the synthesis of biotic compounds. Saladino et al. [4] even argue that formamide may have played a key role in creating and sustaining life on the young Earth, since it can lead to a variety of biologically relevant chemistry such as amino acids, nucleic acids, and sugars. Unfortunately, it is unclear how formamide is formed. One possible formation route is on grain mantles from isocyanic acid (HNCO) hydrogenation (adding hydrogen atoms), to be observed in the gas surrounding hot cores and hot corinos during the warm-up phase of star formation when complex species sublimate [5] (See Figure 2). The alternate formation pathway for formamide is from formaldehyde (H<sub>2</sub>CO) in the gas phase following the reaction:



Observational evidence for the dominant formation route of formamide is contradictory. A nearly linear correlation was observed between the abundances of HNCO and formamide which spans several orders of magnitude in molecular abundance and stellar mass [6][7]. This suggests that the two molecules are chemically related. Observations by Coutens et al. [8] of IRAS 16293-2422 showed that the deuterium fraction in HNCO and  $\text{NH}_2\text{CHO}$  in this solar-mass star-forming region are very similar, indicating a chemical link. On the other hand, Codella et al. [9] observed shocked gas (where high velocity gas collides with the surrounding low velocity gas) near L1157-B1, a solar-like protostar, and found that formamide could be made efficiently in this gas from  $\text{H}_2\text{CO}$ .

*“We found that the morphology and velocity structure of HNCO and  $\text{NH}_2\text{CHO}$  were almost identical.”*

Laboratory studies show that the dominant formation route, either from HNCO in the ice or from  $\text{H}_2\text{CO}$  in the gas, is not completely clear. Recent lab work by Kaňuchová et al. [10] showed that formamide can be formed in ices by cosmic ray irradiated HNCO, but the amount of HNCO formed is not high enough to match observations. Another laboratory study by Noble et al. [11] found that hydrogenating HNCO did not lead to formamide in large quantities and Barone et al. [12] found that gas phase reactions (from  $\text{H}_2\text{CO}$ ) can make significant amounts of formamide.

In my previous work, I studied emission extent, peaks, and velocity structure between HNCO and formamide in the high-mass star-forming region G35.20-0.74N [13]. In G35.20-0.74N B, a high-mass protostellar system potentially surrounded by a Keplerian disk, we found that the morphology and velocity structure of HNCO and  $\text{NH}_2\text{CHO}$  were almost identical, and the velocity structure differed by less than 0.5 km/s. While this is convincing evidence for HNCO as the dominant precursor in this source, we could not rule out  $\text{H}_2\text{CO}$  as a precursor because these observations did not cover any  $\text{H}_2\text{CO}$  lines for comparison.

I have recently performed a pilot study [14] using ALMA observations of very high mass Otype (proto) stars, searching for observational evidence that either HNCO or  $\text{H}_2\text{CO}$  is the dominant predecessor to formamide. In this study, I analysed the spatial extent, kinematics, and molecular abundances of formamide and compared them to HNCO and  $\text{H}_2\text{CO}$  in the gas in three high-mass star-forming regions. The result of my analyses was inconclusive, with the spatial extent of formamide being more similar to HNCO, but the velocity structure more similar to  $\text{H}_2\text{CO}$ . Additionally, there were abundance correlations between all three pairs of species, indicating that this may not be a good test of their chemical relationship.

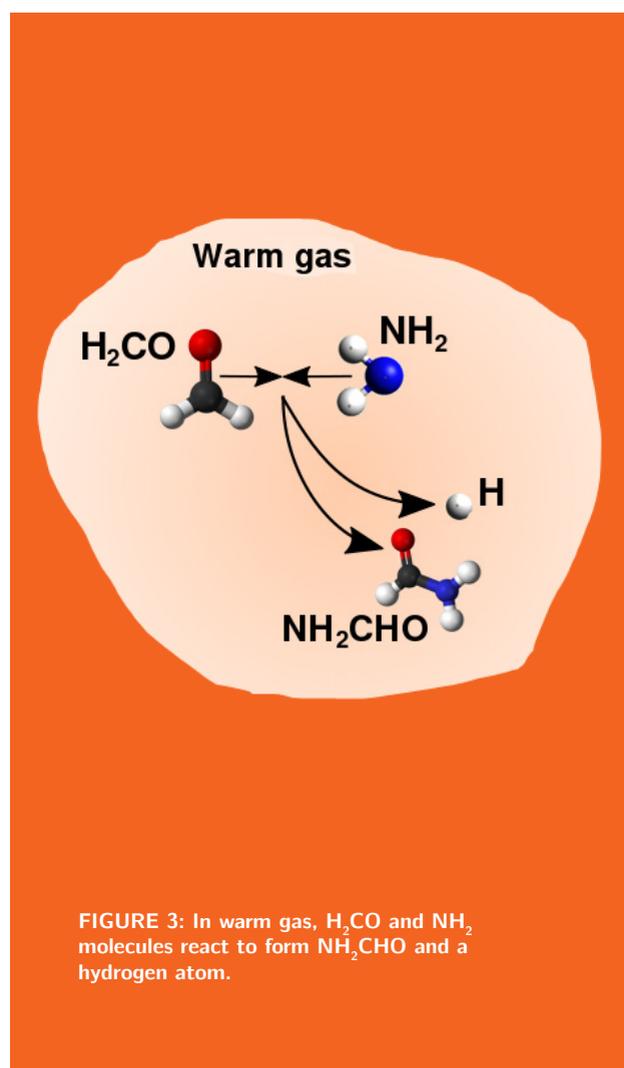


FIGURE 3: In warm gas,  $\text{H}_2\text{CO}$  and  $\text{NH}_2$  molecules react to form  $\text{NH}_2\text{CHO}$  and a hydrogen atom.

### Future work

The James Webb Space Telescope (JWST) will be launched early next year and early science observations of ices in star-forming regions are planned. This is a space-based infrared telescope that would be able to detect molecular species in ice that were previously undetectable. Observing HNCO, H<sub>2</sub>CO and formamide in ices would provide new evidence in the problem of determining the formation route of formamide. The laboratory work of Urso et al. [15] has proposed that formamide can be detected in mid-infrared spectra of ice mantles. HNCO has not yet been detected in ice, but its presence was associated with the “XCN” ice feature at 4.62 μm in infrared observations of interstellar ice [16] [17]. This comes from the assumption that the XCN feature is

*“JWST ice observations will give insight into the ice formation routes for formamide.”*

OCN<sup>-</sup>, which becomes HNCO when it is released into the gas phase and the ion recombines to form a neutral species. Additionally, the ice feature at 6.85 μm has been proposed to be NH<sub>4</sub><sup>+</sup> and, when taken together with the potential OCN<sup>-</sup> feature, leads to the conclusion that these two ions were formed by an acid-base reaction between NH<sub>3</sub> and HNCO.

More work is needed from all three groups of astrochemists. Dedicated ALMA observations of HNCO, H<sub>2</sub>CO and formamide near high- and low-mass protostars will improve upon my pilot study greatly. JWST ice observations will give insight into the ice formation routes for formamide. In the laboratory, more experiments are needed to understand the effects of different astronomical phenomena on the formation of formamide. Theorists need to test grids of models simulating different types of sources and the formation of formamide through different stages of star and planet formation. With the three groups working together on this problem we will soon have a clear understanding of the formation of this key species•

### References:

1. Herbst, E. & van Dishoeck, E. F. 2009, ARA&A, 47, 427
2. Favre, C.; Pagani, L.; Goldsmith, P. F.; Bergin, E. A.; et al. 2017. A&A, 604, L2
3. Pagani, L.; Favre, C.; Goldsmith, P. F.; et al. 2017. A&A, 604, A32
4. Saladino, R., Crestini, C., Pino, S., et al. 2012, Phys. of Life Rev., 9, 84
5. Kahane, C., Ceccarelli, C., Faure, A., & Caux, E. 2013, ApJ, 763, L38
6. López-Sepulcre, A., Jaber, A. A., Mendoza, E., et al. 2015, MNRAS, 449, 2438
7. Mendoza, E., Lefloch, B., López-Sepulcre, A., et al. 2014, MNRAS, 445, 151
8. Coutens, A., Jørgensen, J. K., van der Wiel, M. H. D., et al. 2016, A&A, 590, L6
9. Codella, C., Ceccarelli, C., Caselli, P., et al. 2017, A&A, 605, L3
10. Kaňuchová, Z., Boduch, P., Domaracka, A., et al. 2017, A&A, 604, A68
11. Noble, J. A., Theule, P., Congiu, E., et al. 2015, A&A, 576, A91
12. Barone, V., Latouche, C., Skouteris, D., et al. 2015, MNRAS, 453, L31
13. Allen, V., van der Tak, F. F. S., Sánchez-Monge, Á., Cesaroni, R., & Beltrán, M. T. 2017, A&A, 603, A133
14. Allen, V., van der Tak, F. F. S., López-Sepulcre, A., Cesaroni, R., Sánchez-Monge, Á., Rivilla, V. in prep.
15. Urso, R. G., Scirè, C., Baratta, G. A., et al. 2017, Phys. Chem. Chem. Phys., 19
16. Öberg, K. I., Boogert, A. C. A., Pontoppidan, K. M., et al. 2011. ApJ, 740, 2, 109
17. Boogert, A. C. A., Gerakines, P. A., & Whittet, D. C. B. 2015, ARA&A, 53, 541

**Creatieve software engineer?**

**Hou jij van afwisseling?**

**Zou je je willen specialiseren in Big data toepassingen?**

**Geïnteresseerd in de industrie, verkeer of zorg sector?**

**Ben je goed in programmeren liefst in c++?**

**Achtergrond in Natuurkunde, Informatica of AI?**

Wij hebben vacatures voor zowel ervaren engineers als trainees.

KxA datasolutions is een innovatief bedrijf voortgekomen uit de astronomie, gespecialiseerd in data toepassingen en gevestigd op de grens van Groningen en Friesland. We werken aan veel verschillende dataprojecten. De ene keer houden we ons bezig met slimme datatoepassingen voor het verkeer de andere keer zijn we bezig met de optimalisatie van een fabriek of helpen we mee aan de ontwikkeling van een innovatieve windmolen of analyseren we onverwachte uitval in een fabriek.

Geïnteresseerd? Kom dan eens kennismaken.

Geen auto? Wij kunnen zorgen voor vervoer.



**Geïnteresseerd? Bel of mail!**

**{kxa}**  
DataSolutions

**Wilma Mulder**  
**mulder@kxa.nl**  
**tel. 06 15347819**

## Theory in Support of Experiments on Atoms and Molecules

AUTHOR: ANASTASIA BORSCHEVSKY

Theoretical support is very important and often crucial for the success of experiments performed on atoms and molecules. This is especially true in case of experiments on heavy and superheavy elements, which are challenging due to the low quantities and often very short lifetimes of the investigated atoms. Another field where theoretical input is indispensable is in experiments that strive to achieve very high precision, such as atomic clocks, or any experiment to search for new physical phenomena (physics beyond the Standard Model) using atoms or molecules. Using theoretical models and state of the art computational tools, one can perform high accuracy calculations of various properties needed for success of such experiments.

**T**heoretical input can contribute at all stages of an experiment, starting with initial planning of the measurements and the experimental design. In a spectroscopy experiment, theoretical prediction of the energy of a given transition allows the experimentalists to focus on a certain range in their measurements, and to avoid broad wavelength scans. In the next step, theoretical input is often required to extract the necessary information from the measurements. For example, using atomic or molecular hyperfine structure spectroscopy one can obtain important information about the nucleus (nuclear magnetic and quadrupole moments and nuclear size) from the measured transition energies combined with theoretical predictions of electronic structure parameters. Once an experiment is successful, scientists turn to theory for comparison of the measured value with the theoretical predictions, for an additional confirmation (and also as a test of different theoretical models and their predictive power). Theory is also important in the interpretation of the experimental results. Knowledge of the electronic structure of a given system can assist in explaining its physical properties. For example, we can use theory to explain different chemical behaviour of two very similar molecules.

### Theory preceding experiments

Finally, one can perform theoretical investigation in cases where experiment is not (yet) possible. For example, even though an element with atomic charge  $Z=120$  has not even been discovered yet, its atomic properties, such as ionisation potential and transition energies have been already calculated with very high accuracy. These calculations provide us with information on properties and trends where no experiment is available and they also might be useful in future experiment. In this case, the advantage of theoretical research is that it is not limited by practical considerations, and there are no atomic or molecular systems or properties that are beyond our reach.

*“Theoretical input is often required to extract the necessary information from the measurements.”*

## Relativistic calculations

Of course, in order to be useful in experiments (or even in purely theoretical investigations) theoretical predictions should be reliable and thus based on very accurate calculations. In particular, when dealing with heavy and superheavy elements, or when one is interested in properties where relativistic effects are important, the calculations should be based on the relativistic Dirac Hamiltonian, rather than on the standard Schrödinger equation. Using a non-relativistic framework in such calculations may lead not just to low accuracy but also to qualitatively wrong results, such as a misidentification of the ground state of the system. Another important parameter that determines the quality of any calculation is treatment of electron correlation, or instantaneous interaction between the electrons.

## Electron correlation

A number of computational methods were developed in order to describe electron correlation; some of these methods are extremely accurate (but unfortunately also very computationally expensive). How can one determine the accuracy of a prediction of a property that has never been measured before? To continue with the example of element 120 mentioned above, alongside the calculations for this system we perform the same calculations for the properties of its lighter homologues (elements situated in the same column of a Periodic Table). We expect the method to perform on a similar level for these similar systems. We can then compare the calculated properties of the lighter atoms to the available experimental data, and thus assess the accuracy of our results and the reliability of our predictions for the heaviest element. We can also assess the sources and magnitude of possible errors from the knowledge of the approximation that we make in our calculations.

## Beyond the Standard Model

In our research group at the VSI we specialise in high accuracy theoretical calculations, focusing on research in the field of heavy and superheavy elements and search for physics beyond the Standard Model with atoms and molecules. All the calculations are carried out in relativistic framework and we use state-of-the-art methods for treatment of electron correlation, which allows us to achieve benchmark accuracy. A major part of our theoretical work is done in collaboration with experimental groups here in the Netherlands and around the world.

*“Using a non-relativistic framework in such calculations may lead not just to low accuracy but also to qualitatively wrong results.”*

## Electron electric dipole moment

A large part of our work is currently centered around the experiment to measure the electron electric dipole moment (eEDM) that is currently prepared in Groningen in collaboration with VU Amsterdam. The Standard Model of particle physics (SM) predicts the electron to have a vanishingly small dipole moment, but other theories that attempt to go beyond the SM and resolve its shortcomings predict a

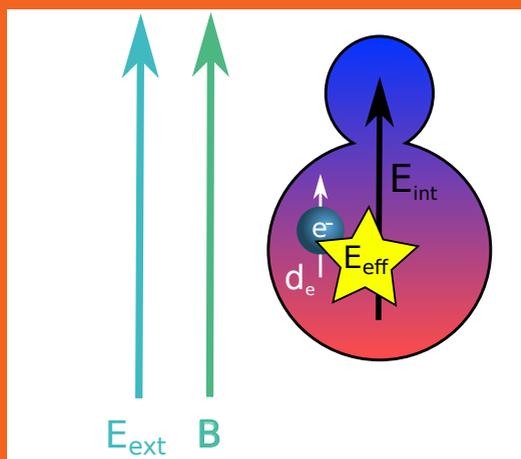


FIGURE 2: The polar BaF molecule has an internal electric field,  $E_{int}$  (black arrow). In an external electric and magnetic fields the molecule and the eEDM (white arrow) will align with the direction of the applied fields which is an essential feature of the possibility of an eEDM measurement. The yellow star represents the interaction between  $d_e$  and  $E_{int}$ , the strength of which is denoted the effective electric field,  $E_{eff}$ .  $E_{eff}$  cannot be measured in experiment and has to be calculated using highly accurate quantum chemical methods.

*“There are many exciting opportunities in the group for Bachelor and Master research projects.”*

much larger eEDM. The predictions vary from model to model and thus a measurement of this property would allow us to test these theories. The experiment at Groningen will be carried out on a beam of cold and slow BaF molecules (Barium monofluoride - ed.), and considerable theoretical input is needed for its success. In one of the stages of the experiment the molecules will be laser cooled; planning this stage requires knowledge of accurate spectroscopic parameters of the BaF molecules, which we have calculated recently with high precision. Once the experiment is completed, theory will also be required to extract the magnitude of the electron EDM (or the upper limit on it) from the measurements. What is measured in practice is a small energy shift  $\Delta E_{eEDM}$  due to the interaction of the eEDM ( $d_e$ ) with the internal effective field ( $E_{Eff}$ ) of the molecule:

$$\Delta E_{eEDM} = d_e E_{Eff}.$$

This effective electric field cannot be measured experimentally and has to come from theory. The accuracy of the calculated  $E_{Eff}$  will influence the accuracy of the extracted eEDM, which is why we are currently working hard on providing the most precise value possible within the current methods for this property. Some theory development and software implementations were required to make these calculations possible, and we are looking forward to using them to help interpret the results of the experiment.

#### Multiple topics

Besides the investigations of BaF in the context in the framework of the experiment for electron EDM, there are many other topics that we are currently working on using similar accurate computational approaches. Some examples are calculations of spectra of highly charged tin ions, needed to investigate tin plasma produced at ARCNL (research centre connected to ASML), studies of spectra and properties of superheavy elements, in collaboration with experimental teams from Germany and Japan, and investigations of atoms and molecules in the context of search for variation of fundamental constants and parity violation phenomena. Thus, there are many exciting opportunities in the group for Bachelor and Master research projects•

# Advanced CT Imaging for Accurate Proton Therapy Planning

AUTHORS: JOANNE K. VAN ABBEMA, MARC-JAN VAN GOETHEM, SYTZE BRANDENBURG, EMIEL R. VAN DER GRAAF

New technological developments have improved the quality in treatment of cancer with photons. However, cancer still remains a challenging disease to cure considering the 5 year survival rate of around 60%. The use of protons instead of photons is a next step in the process to increase this survival rate for certain types of patients. Children and patients with tumours in the head and neck region (including eye tumours) can potentially benefit most from proton therapy. Treatment of patients with protons will start at the new Groningen Proton Therapy Centre in 2018. The treatment plans for proton therapy are based on CT imaging with photons, providing information about the interactions of photons with the various tissues in a patient. This photon-based information has to be translated into information that allows the prediction of the range and energy deposition of protons in these tissues. This translation is the topic of a joint research project of KVI-CART and UMCG.

## Protons versus photons

Photons interact with tissue mainly through photoelectric absorption and coherent (Rayleigh) and incoherent (Compton) scattering. The depth dose distribution of photons with therapeutic energies (6-15 MV) in water shows a dose build-up region to a maximum at approximately 1.5 to 2.5 cm depth due to the relatively long range of the forward scattered electrons. After the maximum the dose nearly exponentially decreases with depth due to the exponential attenuation of the photon beam with traversed distance.

Protons predominantly lose energy in small amounts by many Coulomb interactions with the electrons in the tissue and travel along a nearly straight path. The proton energy (and velocity) decreases and the proton energy loss increases towards the end of the proton

path resulting in a relatively sharp energy deposition peak (Bragg peak). Figure 1, which compares the dose profiles of photons and protons with therapeutic energies, indicates that the profile for protons is more suited for delivering a high dose to a tumour while sparing healthy tissue. However, this also involves a large challenge. Although a high dose can in principle be delivered very conform to the tumour due to the steep fall off of the Bragg peak, there is the risk that errors in the positioning of the high dose region lead to a high dose to healthy tissue or to insufficient dose to the tumour. This means that the proton range has to be predicted very accurately, for which it is crucial to correctly translate the photon imaging information into information to predict the proton range.

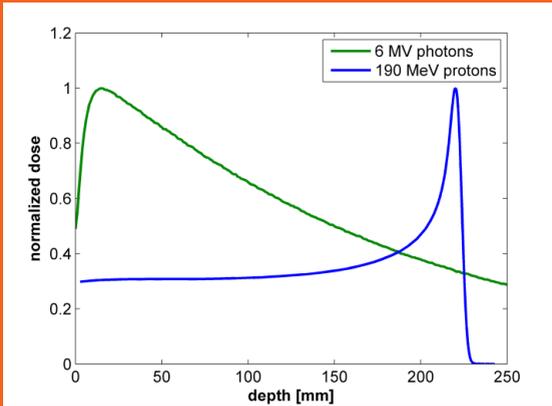


FIGURE 1: Normalised depth dose distributions for 6 MV photons and 190 MeV protons measured in water.

### Prediction of proton range

The proton range can be calculated from the proton stopping power, which is the proton energy loss per distance traversed. The stopping power of a certain material is a function of the proton energy and the material's composition and density and is described by the so called Bethe-Bloch formula. The proton energy is a parameter that is under control by the energy selection system of the cyclotron that delivers the therapeutic proton beam. Information about the stopping power can be deduced from CT imaging. The standard practice is to use a CT image with one detector and one x-ray tube usually at a high voltage of 120 kV. Such a Single Energy CT (SECT) image provides the linear attenuation coefficient in each voxel (small volume element) of the patient for the photon spectrum generated by the x-ray tube. The link to the proton stopping power is then made using an empirical calibration curve in which measured and/or calculated linear attenuation coefficients are correlated with calculated proton stopping powers for a set of materials with well known composition and density (see Figure 2). The SECT calibration is identical for every patient and consequently is insensitive for differences between patients.

In the last decade Dual Energy CT (DECT) imaging has been introduced in the clinic. With DECT, images are acquired at a lower tube voltage (e.g. 90 kV) and a higher tube voltage (e.g. 150 kV) leading to linear attenuation coefficients for a low energy x-ray

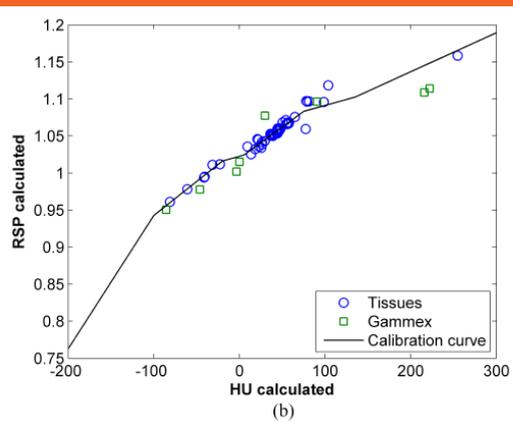
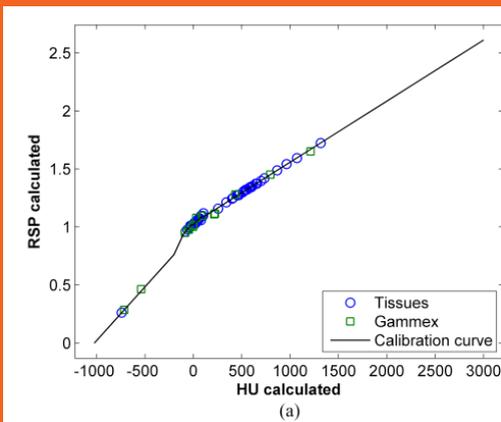


FIGURE 2: a) SECT based calibration curve that correlates the proton stopping power relative to water with the Hounsfield unit H (directly related to the linear attenuation coefficient) of the material (Gammex indicates tissue equivalent materials), b) Enlarged view of the data around water (HU=0).

spectrum and a high energy x-ray spectrum. From these two attenuation coefficients and a theoretical model of the dependence of the attenuation coefficient on the atomic number and the electron density, an effective atomic number and electron density per voxel can be derived. This is possible because of the difference in energy and atomic number dependency of the photoelectric effect and Compton scattering. The effective atomic number and the electron density can then be used in the Bethe-Bloch equation to calculate proton stopping powers and proton ranges. This DECT based proton stopping power prediction is physics-based and patient specific and avoids the use of an empirical calibration curve.

### Experimental SECT-DECT comparison

In the KVI-CART UMCG research project the developed DECT method was extensively tested on a large set of materials that were imaged with both SECT and DECT at the newest generation dual-source DECT scanner at the Radiology department of the UMCG. From these images proton stopping powers were predicted by both the SECT and DECT method. In addition, the proton stopping power was very accurately measured for all the materials using proton beams from the KVI-CART cyclotron. This database of measured proton stopping powers provides a ground truth for the comparison of both methods. From the results in Figure 3 it is evident that DECT outperforms SECT significantly for proton stopping power prediction.

*“This database of measured proton stopping powers provides a ground truth for the comparison of both methods.”*

### In conclusion

Using DECT — instead of SECT — imaging for proton therapy treatment planning seems to be the next step forward in the quest for higher accuracy in proton therapy. Clinical introduction of the method is expected to be realised in the coming years.

To further improve on the quality of the accuracy of proton range prediction KVI-CART and UMCG have recently started a project on the use of proton radiography (2D imaging with protons) as a feedback mechanism for the DECT predicted proton ranges. A comparison between the predicted and the measured proton radiograph will be used to update the prediction from the DECT imaging. Especially in treatment of tumours in the head and neck, with a complex variation between air (oral and nasal cavities) and soft and hard tissues (bones, teeth, fillings), this is expected to increase the treatment quality•

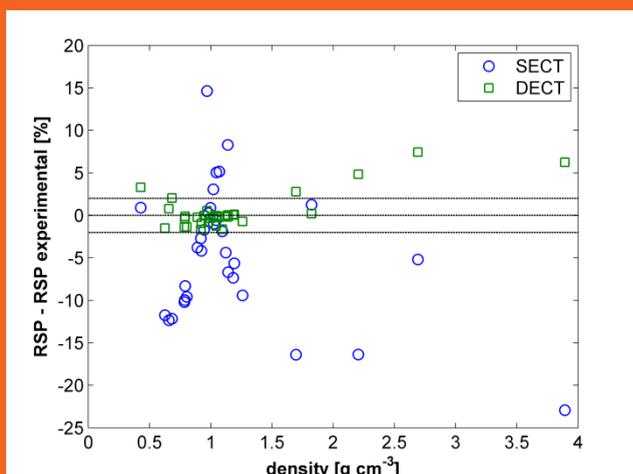


FIGURE 3: Comparison of stopping powers (RSPs) relative to water determined with single energy CT (SECT) and dual energy CT (DECT) with experimental RSPs as a function of mass density for 32 materials. The horizontal lines represent differences of ±2% and 0%, respectively.

## Exploring complex dynamics with Lyapunov exponents

AUTHOR: ALEF STERK

Dynamical systems are mathematical models for everything that moves in time. Simple examples are springs and pendulum clocks. More complicated examples are the atmosphere producing the everyday weather and the celestial bodies comprising the solar system. Such systems are deterministic in the sense that the present “state” of the system completely determines its future. In other words, probability does not play a role. For each system it is necessary to specify what its states are. For example, the state of a pendulum clock is given by the position and velocity of the swinging weight. Newton’s laws then provide a description how these states evolve deterministically in time.

The mathematical theory of dynamical systems aims to study and understand (1) the longterm behaviour of nonlinear deterministic systems, and (2) the qualitative changes in dynamics upon variation of system parameters modelling external influences [2]. Instead of studying individual evolutions, the aim is to obtain a coherent overview of the dynamics by studying the geometric organisation of the product of the state space and the parameter space. In particular, the transition from orderly to complex chaotic dynamics is an important aspect. The theory of dynamical systems enjoys a lot of interplay between different branches of mathematics, such as analysis, geometry and topology, and numerical mathematics. In this article, I will illustrate by means of a simple example how we use dynamical indicators such as Lyapunov exponents to explore the dynamics of deterministic systems.

### A population model

As an example of a dynamical system we will consider a model from mathematical biology which describes the population size of successive generations of

a certain species. The simplest possible model is obtained when one assumes that each individual gives rise to  $r$  individuals in the next generations. In other words, if  $x_n$  denotes the population size at generation  $n$ , then the population size of the next generation is given by the formula

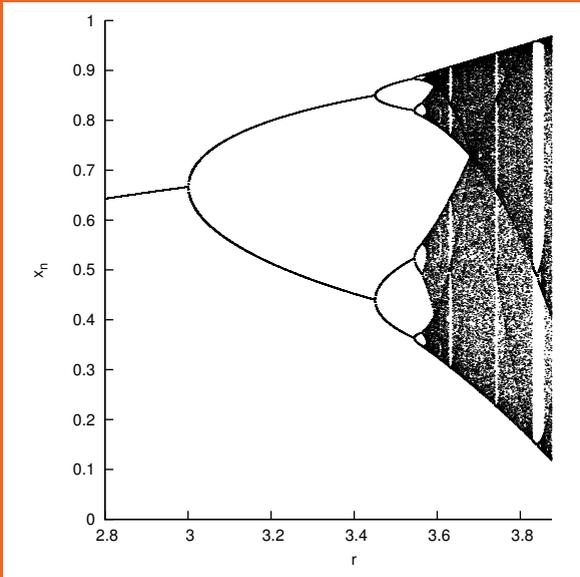
$$x_{n+1} = rx_n.$$

In this model the parameter  $r > 0$  is the growth rate of the population. If the initial population is denoted by  $x_0$ , then the population size at time  $n$  is  $x_n = r^n x_0$ . If  $0 < r < 1$ , then the population decays exponentially fast, whereas for  $r > 1$  the population increases exponentially fast. In the case  $r = 1$  the population remains constant in time. Thus, in this model it is possible to give a complete overview of the dynamics in terms of the parameter  $r$ .

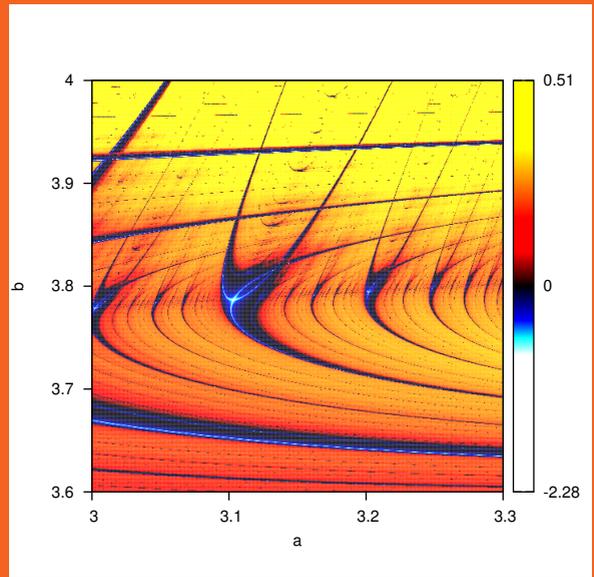
A more realistic model, which takes overpopulation into account, is given by the so-called *logistic model*:

$$x_{n+1} = rx_n(1 - x_n), \quad (1)$$

where  $0 \leq r \leq 4$ . This model was studied extensively



**FIGURE 1:** Bifurcation diagram of the logistic model.



**FIGURE 2:** The Lyapunov exponent plotted as a function of  $a$  and  $b$  for the logistic model with  $r=a, b, a, b, \dots$

and popularised by Robert May in the 1970s [5]. By an induction argument it follows that  $0 \leq x_0 \leq 1$  implies that  $0 \leq x_n \leq 1$  for all  $n \geq 1$ . In particular, this implies that exponential growth is no longer possible in this model.

An overview of the dynamics can be obtained by means of a so-called *bifurcation diagram*, which visualizes the values of  $x_n$  of a system visited or approached asymptotically as a function of a parameter of the system. For a fixed value of  $r$  a sequence of 1500 successive  $x_n$ 's of the logistic model are computed of which the last 150 points are plotted. Then the parameter  $r$  is increased by a small step and the procedure is repeated. The resulting diagram, which is shown in Figure 1, shows the bifurcations (literally: forking) of the periods of stable orbits from 1 to 2 to 4 to 8 and so on. Each of these bifurcation points is a so-called period-doubling bifurcation.

An extension of the logistic model was proposed in [8] by allowing “seasonal changes” of the growth rate parameter  $r$ . We will consider the situation in which the parameter  $r$  can attain two distinct values  $a$  and  $b$  according to some deterministic rule. Now we effectively have two parameters that can be varied, and therefore exploring the dynamics as function of these parameters becomes a more challenging task. Bifurcation diagrams in one parameter while keeping the other fixed, such as Figure 1, do not give a coherent

picture. Such diagrams also become less useful for higher dimensional systems and continuous-time systems. Therefore, we need better tools. One such tool will be introduced next.

### Lyapunov exponents

For  $r$  sufficiently large the dynamics of the logistic model (1) can become chaotic. The key feature of chaotic dynamics is sensitive dependence on initial conditions: two evolutions starting at nearby initial states quickly drift apart. For a 1-dimensional dynamical system of the form  $x_{n+1} = f(x_n)$  we define the so-called Lyapunov exponent as

$$\lambda(x_0) = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=0}^{n-1} \log |f'(x_k)|$$

Using Birkhoff's theorem from ergodic theory [3] it can be proven that the limit  $\lambda$  exists and is independent of  $x_0$  for almost all  $x_0$ . The Lyapunov exponent gives the rate of exponential divergence from a perturbed initial condition  $x_0$  and hence is a measure for chaos.

A negative Lyapunov exponent indicates periodic dynamics, whereas a positive exponent indicates chaotic dynamics. This offers a graphical tool of studying how the dynamics of a system depends on parameter values. We will illustrate this using the logistic model with seasonal variations. We will

*“Lyapunov diagrams are an important tool in the identification of chaotic dynamics and the bifurcation sequences leading to it.”*

assume that the parameter  $r$  switches between two values  $a$  and  $b$  at each time step. So in equation (1) we replace  $r$  by  $r_n$  which is given by the sequence  $a, b, a, b, a, b, \dots$ . Figure 2 shows a graph of the magnitude of the Lyapunov exponent  $\lambda$  as a function of  $a$  and  $b$  and reveals an intricate shrimp-shaped structure in the parameter plane. Replacing  $r_n$  by the sequence  $a, a, b, a, a, b, \dots$  gives the diagram of Figure (3), which reveals a very different structure. Therefore, Lyapunov diagrams are an important tool in the identification of chaotic dynamics and the bifurcation sequences leading to it.

### Conclusion

The research unit *Dynamical Systems, Geometry, and Mathematical Physics* at the Johann Bernoulli Institute has a longstanding tradition in the study of nonlinear deterministic systems. We develop and implement computational tools, such as power spectra, Lyapunov exponents, entropies, and fractal dimensions. These tools help to distinguish different types of dynamics. In this article I illustrated one of these techniques using a simple example. For  $n$ -dimensional systems there is a *spectrum* consisting of  $n$  Lyapunov exponents. The first two or three exponents already give a very good indication on the type of dynamics. We have used the technique in more complex dynamical systems including population models and climate models [1, 4, 6, 7]•

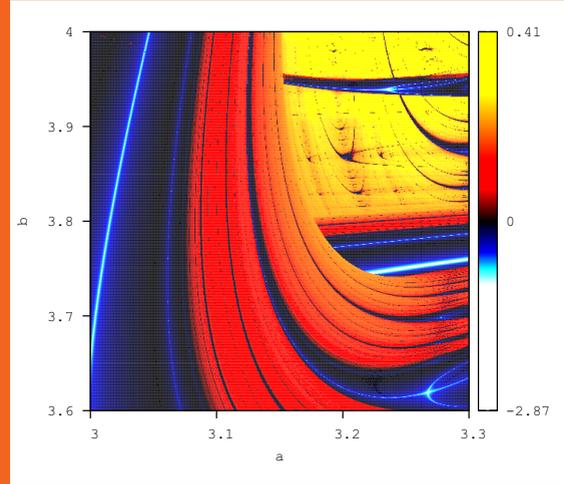


FIGURE 3: As Figure 1, but for  $r=a, a, b, a, a, b, \dots$

### References

- [1] H.W. Broer, H.A. Dijkstra, C. Simó, A.E. Sterk, R. Vitolo. The dynamics of a low-order model for the Atlantic Multidecadal Oscillation. *Discrete and Continuous Dynamical Systems – Series B*, 16, pp. 73-107, 2011.
- [2] H.W. Broer, F. Takens. *Dynamical Systems and Chaos*. Springer, 2011.
- [3] G.H. Choe. *Computational Ergodic Theory*. Springer, 2005.
- [4] S. Garst, A.E. Sterk. The dynamics of a fold-and-twist map. *Indagationes Mathematicae*, 27, pp. 1279-1304, 2016.
- [5] R.M. May. Simple mathematical models with very complicated dynamics. *Nature*, 261, pp. 459-466, 1976.
- [6] D.L. van Kekem, A.E. Sterk. Travelling waves and their bifurcations in the Lorenz-96 model. *Physica D: Nonlinear Phenomena*, 367, pp. 38-60, 2018.
- [7] A.E. Sterk, R. Vitolo, H.W. Broer, C. Simó, H.A. Dijkstra. New nonlinear mechanisms of midlatitude atmospheric low-frequency variability. *Physica D: Nonlinear Phenomena*, 239, pp. 702-718, 2010.
- [8] J. Rössler, M. Kiwi, B. Hess, M. Markus. Modulated nonlinear processes and a novel mechanism to induce chaos. *Physical Review A*, 39, pp. 5954-5960, 1989.

Do you pursue a  
technical master's  
degree?

apply for the  
ASML Technology  
Scholarship

receive 2 years  
of financial  
support



follow an  
extensive  
development  
program

and get to know  
ASML from  
the inside

ASML pushes technology further, to print microchips features that are finer, to accelerate artificial intelligence, to make robots understand humans, to let robots help in healthcare. Interested?

Apply for the ASML Technology Scholarship before April 13th.  
[workingatasml.com/scholarship](http://workingatasml.com/scholarship).

**ASML**

Be part of progress

# Jumping in the Solid Phase: Perovskites for Solar Cells and Beyond

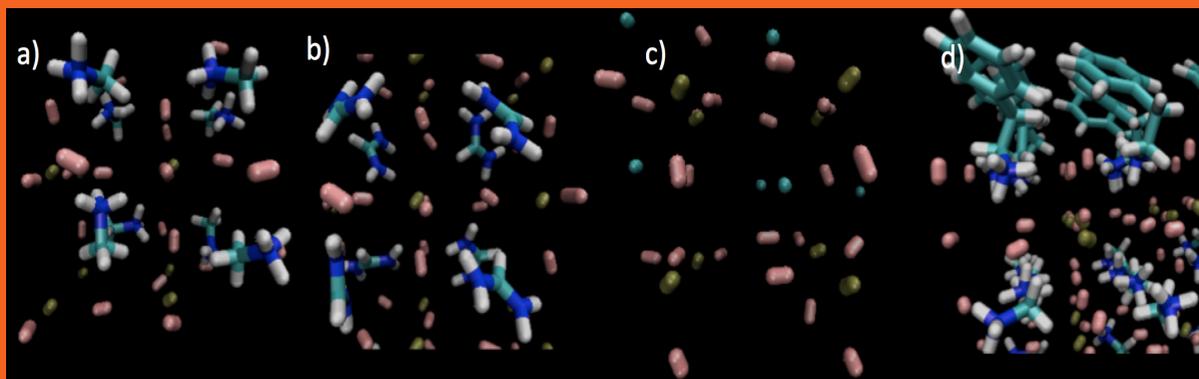
AUTHOR: THOMAS JANSEN

Silicon is currently dominating the market for solar cells. While production prices are dropping and the installation of solar panels is growing faster than ever, the emission of CO<sub>2</sub> is still increasing.

In 2009 a new dream material holding the promise of lightweight, easily processable and efficient solar cells was reported. This material is a mixture of inorganic (atomic) and organic (molecular) ions. In the meantime, research cells of this type of material has reached efficiencies beyond 22%. Still, the fundamental physics behind this efficiency is poorly understood. It is for example still disputed

whether the material is a direct or indirect bandgap semiconductor. The role of the molecular ions is heavily discussed. Furthermore, the properties of new materials with other molecular ions are currently explored.

The original organometal halide perovskite solar cell material [1] is made of lead, iodine, and



**FIGURE 1:** Snapshots of structures seen in molecular dynamics simulations of a) lead iodine methylammonium (PbI<sub>3</sub>CH<sub>3</sub>NH<sub>3</sub>), b) lead iodine formamidinium (PbI<sub>3</sub>CH(NH<sub>2</sub>)<sub>2</sub>), c) lead iodine cesium (PbI<sub>3</sub>Cs), and d) lead iodine methylammonium perovskite covered with a benzeneethan ammonium layer. The colour code: lead is golden, iodine is pink, cesium is dark green, carbon is cyan, nitrogen is blue, and hydrogen is white.

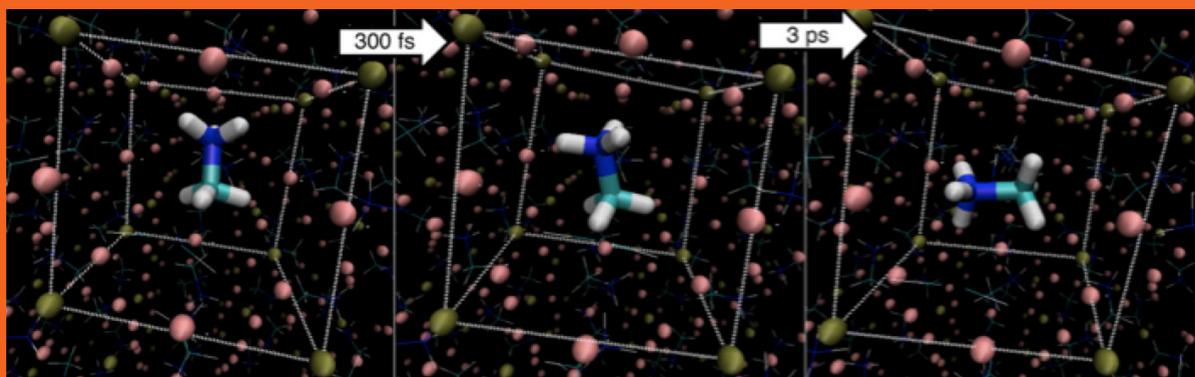
methylammonium (see Figure 1). One of the fascinating properties of the molecular ions in this material is that they have a large dipole moment and they are able to rotate. Initial reports by indirect nuclear magnetic resonance measurements suggested that this rotation was essentially free [2]. However, speculation started that the molecular ions could actually form domains, where the methylammonium would all point in the same direction leading to ferroelectricity [3] and the potential implications for the solar cell performance were explored [4]. The unique properties of the original organometal halide perovskite solar cell materials can be explored not only in solar cell materials, but also in field effect transistors, LEDs, and thermoelectric devices. However, fundamental understanding of the origin of these unique properties is crucial for proper device optimisation.

The rotation of the organic ions can be measured directly using an ultrafast two-dimensional infrared spectroscopy technique, which essentially allows tagging a particular molecule in the material at one point in time and femtoseconds later probe how much the molecule rotated [5]. This could be combined with molecular dynamics simulations modeling of the dynamics of the material based on solving Newton's equations for the atoms, assuming interactions as the Coulomb and van der Waals type. Both these direct experiments and the molecular dynamics simulations

suggested the existence of two timescales for the rotation of the molecular ions in contrast to the single timescale originally found with the indirect nuclear magnetic resonance measurements (see Figure 2 and 3). By analyzing the molecular dynamics simulation it was possible to identify the two underlying mechanisms of rotation. The fastest type ( $\sim 300$  fs) which was assigned to wobbling-in-a-cone type motion, where the overall direction of the molecular dipole was moving back and forth within a cone with a semi-cone angle of about  $30^\circ$ . The second type of motion involves  $90^\circ$  angular jumps on a much slower (3 ps) timescale ten times slower than the dynamics originally observed through indirect methods [2].

The observation of picosecond timescale dynamics does seem to rule out ferroelectricity playing a major role, at least at room temperature in the original lead iodide material. It is, however, interesting to see if one can modify the dynamics of the ions. Combining ultrafast spectroscopic techniques and molecular dynamics it was possible to show that when replacing part of the iodine atoms with bromine the cube structure in the perovskites was distorted, which resulted in a significant slowdown of the 3 ps jumps [6], but little change in the fast wobbling-in-a-cone type motion.

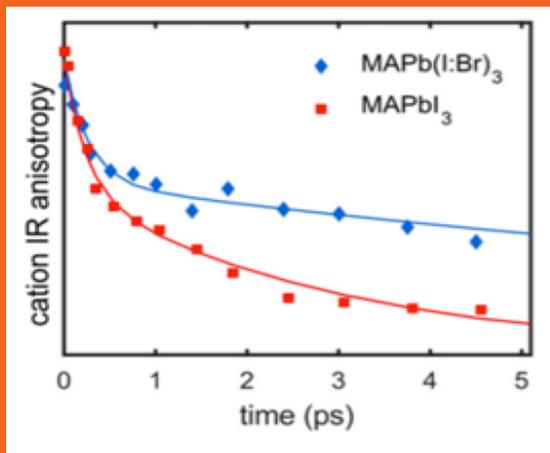
Currently, we are examining how the perovskite material behaves when other ions are incorporated



**FIGURE 2:** Left: Illustration of the 300 fs wobbling-in-a-cone motion and the 3 ps jump motion. The colour scheme is identical to that in Figure 1.

in the material. Interesting effects have been reported when for example cesium or formamidinium (see Figure 1) ions are incorporated in the material. These ions both have much smaller dipole moment than methylammonium, but still, solar cells with high efficiency can be achieved. Larger ions as benzeneethan ammonium have been reported as useful protective coatings increasing the stability of perovskite-based materials, which is also crucial to achieve before industrial applications are possible. The interface between perovskite and hole and electron extraction layers is also important to explore.

The computational methods applied are currently extended beyond molecular dynamics, which only allow studying the dynamics of the nuclei. Electronic structure calculation allows determining the band structure and will, for example, allow solving the discussion of the nature of the band gap and allow a connection with a broad range of experiments [7,8] leading to new design principles•



**FIGURE 3:** The slowdown of the rotation as a fraction of the iodine atoms is replaced with bromine.

## References

- [1] A. Kojima and K. Teshima and Y. Shirai and T. Miyasaka *J. Am. Chem. Soc.* **131** 6050-6051 (2009)
- [2] R. E. Wasylishen and O. Knop and J. B. Macdonald *Solid State Commun.* **56** 581-582 (1985)
- [3] J. M. Frost and K. T. Butler and F. Brivio and C. H. Hendon and M. van Schilfgaarde and A. Walsh *NANO letters* **14** 2584-2590 (2014)
- [4] T. S. Sherkar and L. Jan Anton Koster *Phys. Chem. Chem. Phys.* **18** 331-338 (2016)
- [5] A. A. Bakulin and O. Selig and H. J. Bakker and Y. L. A. Rezus and C. Müller and R. Lovrincic and Z. Sun and Z. Chen and A. Walsh and J. M. Frost and T. L. C. Jansen *J. Phys. Chem. Lett.* **6** 3663-3669 (2015)
- [6] O. Selig and A. Sadhanala and C. Müller and R. Lovrincic and Z. Chen and Y. L. A. Rezus and J. M. Frost and T. L. C. Jansen and A. A. Bakulin *J. Am. Chem. Soc.* **139** 4068-4074 (2017)
- [7] T. S. Sherkar and C. Momblona and L. Gil-Escrig and H. J. Bolink and L. J. A. Koster *Advanced Energy Materials* **7** 1602432 (2017)
- [8] S. Shao and J. Liu and H.-H. Fang and L. Qiu and G. H. ten Brink and J. C. Hummelen and L. J. A. Koster and M. A. Loi *Advanced Energy Materials* **7** 1701305 (2017)

# Vinyl Records

## *The road from studio to loudspeakers*

AUTHORS: RICK VAN VOORBERGEN  
AND ROBERT VAN DER MEER

Over the years, playing music became easier and easier. Most of you grew up listening to cassettes and CD's until you got your very own mp3 player. You were able to download music using all kinds of computer programs to put almost any song on your mp3. Then Apple came along and introduced the iPod with a fancier design and iTunes to download all your favourite music. Eventually the smartphone arrived with streaming applications like Spotify and that is how most of you listen to music nowadays.

**B**ut how did we play music before all these technologies came along? The answer is something which is becoming very popular again these days: phonograph records (a.k.a. vinyl). These black disks — of which probably a bunch are stored in a crate in your parents attic — used to rule the music scene for about 70 years. One would turn on their record player, put the stylus on the spinning vinyl and would enjoy their records until the stylus had run through one side of the record. In this article we would like to explain the steps that take place before one can listen to a record in this way.

We will start explaining how a phonograph record is made, then we will describe how a record is read and finally we will explain how the generated signal is amplified such that the music can be played over loudspeakers.

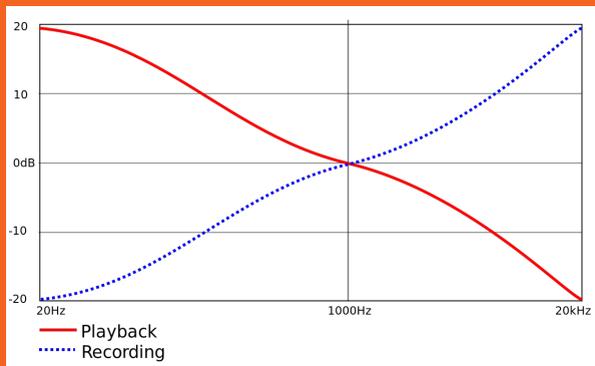
### Vinyl production

First a master recording is made in the studio where the sound is edited to the needs of the producer. In the sound editing stage the recording goes through an equalisation stage. Here the sound editors change the amplitudes of different frequency signals. The recording is modified using the so called RIAA curve, a standardised audio equalisation technique established in 1955 (Figure 1). This is a function of the signal frequency which modifies the amplitude of the incoming signals. In general, one wants to reduce the volume of the lower frequency signals since low frequency signals with large amplitude would require large deviations in the grooves. The inverse of the

RIAA curve is then applied in the amplification of the signal after the signal has been read out by the record player to recreate the original signal. In this process the higher frequency signals are reduced in volume which contain most of the recording noise.

Subsequently a record cutting machine is used to make grooves spiraling inwards in an acetate-coated aluminum disc called a lacquer. The width of a groove is approximately 0.04 – 0.08 mm. The grooves are made varying in deviation from the normal line (the blue dotted line as depicted in Figure 2) corresponding to the frequency of the audio signal. Thereafter, a metal mold called the record master is made by inverting the grooves. The master record then has ridges instead of grooves and using a hydraulic press one can enprint the grooves on the vinyl records.





**FIGURE 1**, The RIAA equalisation curve with in blue the function applied for recording and in red the function applied for playback.

### Reading the grooves

After a record has been bought, the buyer of course wants to listen to the music. But how does one read off the music from the vinyl disk? This can be achieved with a so-called record player. A record player consists of a rotating table called the turntable and an arm with a cartridge attached to its end. The cartridge consists of three main parts: the stylus (better known as the needle), a permanent magnet and a set of coils. To read the grooves, one now places the vinyl on the turntable and let the vinyl rotate with the appropriate number of revolutions per minute (rpm). The so-called long playing records with a diameter of 30 cm are compatible with  $33\frac{1}{3}$  rpm and the smaller records with a diameter of 17.5 cm are compatible with 45 rpm. One places the arm over the vinyl and slowly drops the stylus onto the record. The stylus will quickly land in one of the grooves and will start to follow the track. The grooves make the stylus oscillate with the same frequency as the cutting machine which cut the grooves. In this way the movements that the cutting arm made whilst recording the master onto the vinyl record are 'reproduced'. In most cartridges the permanent magnet is attached to the end of the stylus and a set of coils is placed next to it. This is called a moving magnet cartridge (MM). Now the vibrating stylus will let the magnet oscillate next to the coils causing a magnetic flux-change within the coils. By means of electromagnetic induction an electric signal is generated. One can also have a more expensive moving coil cartridge (MC) in which the coils are attached to the stylus and the magnet remains stationary.

To put it in a more mathematical way, we denote the deviation of the groove from the normal line by  $x(t)$  and the radial distance of the stylus from the center of the turntable by  $r(t)$ . The radial velocity of the needle is then given by

$$v(t) = \frac{dx}{dt} + \frac{dr}{dt}$$

In practice the second term of this expression will in general be negligible compared to the first since the pickup arm will move inwards slowly. So we can say that the output voltage generated by the stylus movement is given by:

$$U(t) = kv(t) = k \frac{dx}{dt}$$

Where  $k$  is the conversion factor called the responsivity of the cartridge. Its value is in general between 0.1-1 mV s/cm.

As an example consider a sine wave signal of frequency  $f$  and amplitude  $A$ . The offset displacement will be of the form

$$x(t) = A \sin(2\pi ft)$$

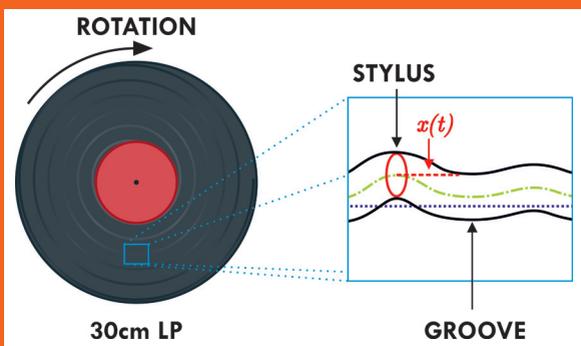
And so its velocity and acceleration are given by

$$v(t) = 2\pi f A \cos(2\pi ft), a(t) = -(2\pi f)^2 A \sin(2\pi ft)$$

A 1kHz wave with an amplification of +20 dB will have a maximal displacement from the normal of about 80 microns and a maximal acceleration of about  $3\text{km/s}^2$ . This is about 320 times bigger than the gravitational acceleration on Earth!

### Preamplification

The signal that leaves the phono cartridge is now being transported to an amplifier. An amplifier increases the voltage amplitude of incoming signals such that the outgoing signal can drive a loudspeaker. Amplifiers are designed to operate for optimised performance when incoming signals have a certain 'nominal' (i.e. standard) level. The standard for consumer audio is the so-called 'audio line level'. To give an example, a



**FIGURE 2:** Schematic view of a groove and the position of the stylus. The blue dotted line in the center denotes the normal line.

CD player that one connects to an amplifier gives an output at audio line level, which is 316 mV. Since the input level of the amplifier matches the output level of the CD player, the device will perform well.

In contrast, the output level of a phono cartridge is 5 mV for a moving magnet cartridge and about a tenth of that for a moving coil cartridge. In terms of voltage, it is therefore not possible to connect the turntable directly to an amplifier.

This brings us to the preamplifier or phono stage. To be able to talk about preamplification, we first need to define the ‘amount of amplification’, which is in terms of gain. The voltage gain in decibels for a device that amplifies a signal of voltage  $V_{in}$  to voltage  $V_{out}$  is defined as

$$\text{gain} = 10 \cdot \log \left( \frac{V_{out}}{V_{in}} \right)^2 \text{ dB}$$

To bring the voltage that the MM cartridge produces to the audio line level of 316 mV, there needs to be a gain of

$$\text{gain} = 10 \cdot \log \left( \frac{316}{5} \right)^2 = 41 \text{ dB}$$

for an MC element, the gain is either 51 dB or 61 dB, depending on the cartridge type. It is therefore



important to have a preamp that matches the cartridge. Some more expensive phono stages are adjustable and can be used for most of the cartridges around.

The preamp has another function. Previously we described that the audio on a vinyl record has been equalised using the RIAA standard curve. Inside the preamp the opposite equalisation takes place, such that the original sound as recorded by the artist in the studio will be restored. If this equalisation would not have been applied, the bass tones would be absent and all the tones in the higher spectrum would sound too loud.

There are three ways of preamplification. Some record players – mostly the cheaper ones – have a preamplifier built in. The output signal is then at line level and can be connected to an amplifier (or it even has a loudspeaker inside). Another way is to use an amplifier that has a preamp built inside. This input will be labelled as ‘phono’ and provides the standard 41 dB gain and the RIAA equalisation. Alternatively, the turntable can be connected to a separate preamp device and then to a ‘regular’ line input on the amplifier.

Summarizing, the signal that comes out of the turntable is very weak and has practically no bass tones and very loud treble tones. Therefore a preamplifier or phono stage is added to the road from vinyl to loudspeaker. In that way the signal’s voltage will be increased and the sound will be equalised to be exactly like it was back in the studio. A preamp can be either built in the turntable, built inside an amplifier, marked as ‘phono’, or it can be a separate device.

### Listening to music

After being preamplified, the audio signal will be boosted by the amplifier once more, to be strong enough to drive loudspeakers. Finally the sound has made its way from the artist in the studio to your loudspeakers and into your ears at home. Enjoy your music! •

### References

[https://www.st-andrews.ac.uk/~jcgl/Scots\\_Guide/iandm/part12/page2.html](https://www.st-andrews.ac.uk/~jcgl/Scots_Guide/iandm/part12/page2.html)

# Brainwork: Count Count

The editors of the periodiek stole a very important message:

8616404 3437296 1544623 5221667 1749601

We didn't want to spoil it for you, so we made it a puzzle to find out what the message is.

You can solve it using the following hints:

- A = 1595959
- B = 4787877
- C = 4363631
- D = 3090893
- E = 9272679
- I = 7818037
- L = 3454111
- M = 362333
- N = 1086999
- O = 3260997
- P = 9782991
- R = 9348973
- S = 8046919
- T = 4140757
- U/V = 2422271

Of every word in the message, the values of the letters in that word are added and only the last seven numbers of the resulting sum are given.

For example for READ PERIODIC we would give you:  
3308504 4756238  
Because the sum yields these values:

$$\text{READ} = 9348973 + 9272679 + 1595959 + 3090893 = 23308504$$

$$\text{PERIODIC} = 9782991 + 9272679 + 9348973 + 7818037 + 3260997 + 3090893 + 7818037 + 4363631 = 54756238$$

The encrypted message is:  
8616404 3437296 1544623 5221667 1749601

What was the original message?

## Previous Brainwork

The solution to the previous brainwork puzzle is given to the right. Thanks again to Johan and Helena for making that puzzle!

The people who sent in the right solutions were:

Thomas ten Cate and Eric Jager.

FALSE	FALSE	TRUE	TRUE	FALSE
TRUE	TRUE	TRUE	TRUE	TRUE
FALSE	FALSE	TRUE	FALSE	FALSE
FALSE	TRUE	FALSE	TRUE	FALSE
FALSE	TRUE	TRUE	TRUE	TRUE
FALSE	TRUE	TRUE	FALSE	FALSE

τ	τ	λ	π	π
λ	π	κ	λ	κ
τ	τ	κ	π	τ
κ	κ	π	κ	τ
κ	π	λ	λ	π
λ	λ	π	κ	κ

# Cream puffs

Tired of eating cream puffs from the freezer? In for a treat that doesn't take hours to make? Need ammo for your catapult? Make these cream puffs! Only four ingredients are needed for making your own freshly baked puffs. Feel free to fill them with anything sweet or savoury.

## Ingredients

100 grams of wheat flower
75 grams of butter
150 mL of tap water
3 eggs
pinch of salt
can of whipped cream

## Kitchenware

oven
small pot
wooden spoon
mixer or whisk
baking tray
baking paper
pipng bag/ziplock bag

## Recipe

Preheat the oven to 200 °C. Sift the flower if needed. Cut the butter in cubes. In a small pot bring the water, the cubes of butter and a pinch of salt to a boil.

When the butter has melted add all the flower. Stir with a wooden spoon until the dough forms a ball, and doesn't stick to the pan. Press any lumps against the side of the pan to get rid of them. Take the pot of the heat and let it cool a little. Beat the eggs through the dough one by one with a mixer or whisk. The dough will become firm and glossy.

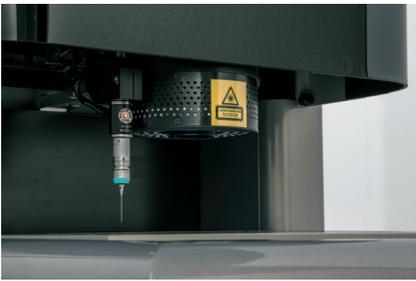
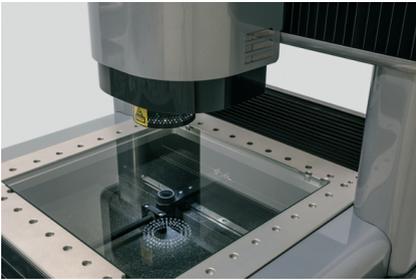
Prepare your baking tray by putting baking paper on it. Transfer the dough to a piping bag or ziplock bag. Cut off a corner and pipe humps of dough onto the baking tray. Be sure to keep enough space inbetween



since puff pastry puffs. Depending on the number of puffs you want to make, you can make the humps bigger or smaller. One batch makes 8 large, 16 medium or 32 small puffs.

Put the baking tray in the middle of the oven and bake the puffs for 10-15 minutes (small) or 20-30 minutes (larger size) until they are lightbrown and cooked. Do not open the oven during baking, this will effect the puffiness of your puffs. The puffs are cooked when they are light and airy and detached from the tray easily.

Fill the puffs with whipped cream after making a hole in the bottom or by gently cutting them in half. Enjoy your homemade cream puffs!•



**Schut Geometrische Meettechniek** is een internationale organisatie met vijf vestigingen in Europa en de hoofdvestiging in Groningen. Het bedrijf is ISO 9001 gecertificeerd en gespecialiseerd in de ontwikkeling, productie, verkoop en service van precisie meetinstrumenten en -systemen.

Aangezien we onze activiteiten uitbreiden, zijn we continu op zoek naar enthousiaste medewerkers om ons team te versterken. Als jij wilt werken in een bedrijf dat mensen met ideeën en initiatief waardeert, dan is Schut Geometrische Meettechniek de plaats. De bedrijfsstructuur is overzichtelijk en de sfeer is informeel met een "no nonsense" karakter.

Op onze afdelingen voor de technische verkoop, software support en ontwikkeling van onze 3D meetmachines werken mensen met een academische achtergrond. Hierbij gaat het om functies zoals *Sales Engineer*, *Software Support Engineer*, *Software Developer (C++)*, *Electronics Developer* en *Mechanical Engineer*.

Je bent bij ons van harte welkom voor een oriënterend gesprek of een open sollicitatiegesprek of overleg over de mogelijkheden van een **stage-** of **afstudeerproject**. Wij raken graag in contact met gemotiveerde en talentvolle studenten.

Voor meer informatie kijk op [www.Schut.com](http://www.Schut.com) en [Vacatures.Schut.com](http://Vacatures.Schut.com), of stuur een e-mail naar [Sollicitatie@Schut.com](mailto:Sollicitatie@Schut.com).



**APPROVE**  
for DeMeet

