

hoch³ FORSCHEN

SCIENCE QUARTERLY

Autumn 2018



TECHNISCHE
UNIVERSITÄT
DARMSTADT

Imprint

Publisher

President of TU Darmstadt,
Karolinenplatz 5,
64289 Darmstadt,
Germany

Editor

Corporate Communication
Jörg Feuck (Editor-in-chief)
Ulrike Albrecht (Graphic Design)
Patrick Bal (Images)

Conceptual design

conclouso GmbH & Co. KG, Mainz,
Germany

Photography (title)

Katrin Binner

Circulation

6.000

Next issue

15th of December 2018

Service for readers

presse@pvw.tu-darmstadt.de

Newsletter subscription

www.tu-darmstadt.de/newsletter

ISSN

2196-1506

Would you like to receive
the next issue of
hoch³FORSCHEN?

Please send an E-Mail to
presse@tu-darmstadt.de



— **1 Chemistry:** New materials with surprising ease — **2 Information science:** Fishing for substance on the internet digitally — **3 Wastewater technology:** The dangers of microplastic in waters — **4 Biology:** Production of sexual attractants strengthens crop protection

Arguments from amongst the noise

Structured decision-making support: The research project "ArgumenText" in the field of Ubiquitous Knowledge Processing has found a way to filter concrete pro and con arguments on any topic from amongst the noise of the internet.

— By Silke Paradowski

Googling for the search term "Nuclear Energy" on the internet yields approximately 268 million hits: Explanations, definitions, lobbying texts, newspaper articles, anecdotes, conspiracy theories. How can someone, for example an investor, seeking real pro and con arguments regarding nuclear power as a decision-making aid, find what they are looking for? The project "ArgumenText" in the field of Ubiquitous Knowledge Processing (UKP) of the Department of Computer Science of TU Darmstadt is aimed at filtering out concrete arguments from voluminous and heterogeneous masses of text. Recently, a demo of the search system came on the scene which has already proven its worth at trade fairs. For example, anyone who researches the subject of "Nuclear Energy" will, after a few seconds, see just under a hundred arguments for and against nuclear power – from a variety of Internet sites. The better CO₂ balance and the efficiency of atomic energy generation are listed here, along with the toxicity and hazardous nature of the substances used and the long periods during which they exude radioactive waste into their surroundings. The respective sources are linked.

"Grammatical structures, contexts and semantics are examined to decide if a statement is an 'argument'."

For this purpose, texts available on the internet are examined by means of neural networks, classified as relevant or not relevant to the search topic, and then tapped for arguments. "Not only are individual words searched, but grammatical structures, contexts and semantics are examined to decide if a statement is an 'argument' or not and whether it is on the pro or con side," explains Dr. Johannes Daxenberger, who works in the team of Professor Iryna Gurevych as one of the two project managers at ArgumenText.

The algorithms behind ArgumenText are under development by the team in the field itself, building on initial experiments that started in 2014 with a body of student essays. "The challenge was to make a system trained on a specific type of text transferable to any kind of text," says second project manager Dr. Christian Stab. "Argumentation in scientific texts, for example, is completely different

than in social media." The team operationalized various models of argumentation theory and taught computer systems to use these models. To optimize the algorithms, the team employed a powerful computer network; a smaller, more powerful computer network that can efficiently index internet-based texts is now used for ongoing operation.

The demonstrator is stable and has recently become publicly available. The project is thus entering the next phase, which will specifically test which applications are particularly promising for the new technology. The main target groups are decision-makers from the business world who must assess whether the use of an innovation is worthwhile, and journalists who must quickly and dependably make their way to the core of a subject in the framework of a search, says Daxenberger. "We think that the system could be used profitably in these areas."

Digital Humanities at the TU Darmstadt

Under the name "Digital Humanities", interdisciplinary collaborations open research-relevant resources in the humanities and cultural sciences using computer-aided methods and make them available digitally. The TU Darmstadt places a significant focus here. Thus, the field of Ubiquitous Knowledge Processing is part of the CEDIFOR (Center for Digital Research in the Humanities, Social and Educational Sciences). The Center helps bridge the gap between humanities research questions and computer-based methods. CEDIFOR builds on the experience, expertise and infrastructure of the LOEWE Digital Humanities focus, in which the TU Darmstadt was also centrally involved.

Information

Ubiquitous Knowledge Processing

Prof. Dr. Iryna Gurevych

E-Mail: gurevych@ukp.informatik.tu-darmstadt.de

Dr.-Ing. Johannes Daxenberger

Email: daxenberger@ukp.informatik.tu-darmstadt.de

Dr.-Ing. Christian Stab

Email: stab@ukp.informatik.tu-darmstadt.de

www.informatik.tu-darmstadt.de/ukp

www.argumenttext.de



Photo: Katrin Binner

Dr. Johannes Daxenberger, Dr. Christian Stab and Dr. Tristan Miller (left to right), together with an international research team, are developing new methods for automatic recognition of arguments in large text sources.

For validation purposes, the participating scientists are currently preparing the method for use with German-language texts as well. Now, ArgumenText speaks only English, works with a text corpus from the year 2016 and works best with technical queries. This will soon change. It will also be possible to search in real time in the ever-growing number of texts on the internet.

Currently, the algorithm sorts statements by how reliably they can serve as arguments. Scientists are working for aggregation of the arguments toward users, presenting them according to themes. "This is obvious from an application perspective, but certainly not trivial from a technical point of view," says Stab. Argument

mining, the recognition of linguistic arguments by means of computer science, is becoming ever more important and visible, say Daxenberger and Stab, in the research of Digital Humanities. The TU was active in this area early on. "Our working group has well and visibly established the TU in the field of argument mining," says Professor Iryna Gurevych, head of the UKP. For this purpose, the interdisciplinary team works with the TU Department of Social and Historical Sciences, as well as with other universities from the network of Rhine-Main universities.

The author is an editor at Corporate Communications of TU Darmstadt.

Publications

Stab, Christian and Daxenberger, Johannes and Stahlhut, Chris and Miller, Tristan and Schiller, Benjamin and Tauchmann, Christopher and Eger, Steffen and Gurevych, Iryna:

ArgumenText: Searching for Arguments in Heterogeneous Sources.

[Online-Edition: <http://www.aclweb.org/anthology/N18-5005>]

In: Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: System Demonstrations. 2018, New Orleans, Louisiana "

ArgumenText

The project ArgumenText is funded by the Federal Ministry of Education and Research (BMBF) within the framework of the VIP + program under grant number 03VP02540 with 1.5 million euros. The project is supported by a special offer of the Capitalization of the TU Darmstadt. Several doctoral and research projects are linked to the project. ArgumenText runs from 2017 to 2020. If you'd like to try it, the public demonstrator can be found under

www.argumentsearch.com.

Microplastics in the river

More and more plastic particles are polluting the environment. In the fields of wastewater technology and wastewater management, research teams are investigating the extent to which industry is involved in microplastic pollution.



Photo: Katrin Binner

Determining microplastic in industrial wastewater: Prof. Markus Engelhart, Prof. Susanne Lackner, Luisa Barkmann and Hajo Bitter.

Information

Department of Wastewater Management

Prof. Dr. Susanne Lackner
Email:
s.lackner@iwar.tu-darmstadt.de

Department of Sewage Technology

Prof. Dr.-Ing. Markus Engelhart
Email: m.engelhart@
iwar.tu-darmstadt.de
www.iwar.tu-darmstadt.de

— By Uta Neubauer

Plastics have become an integral part of our everyday lives. This leaves its footprints in the environment. In addition to carelessly thrown away bags, cups and other plastic waste, pollution with microplastics is increasingly coming into focus. First, the small particles were discovered in oceans; then they were found in lakes and rivers, and eventually in soil. "Plastic particles are everywhere," says Luisa Barkmann, a doctoral student in the field of wastewater technology at the TU Darmstadt. In her Master's thesis, she dealt with microplastics in municipal sewage treatment plants. Now she is dedicated to industrial wastewater. She takes a close look, above all, at

plastic-producing and processing companies in her doctoral thesis: At which stages of the value chain and through which channels do plastic particles enter the environment? And what is the share of industry in the overall burden?

As part of the joint project EmiStop, launched at the beginning of the year, the Darmstadt-based research teams are analysing industrial wastewater to calculate their share of microplastics. Not an easy task, because even sampling is a challenge, says Barkmann. For each company, she had to think of an individual strategy, since the companies differ not only in their production processes, but also in their

channel systems and water management. Many do not even know how much wastewater is generated in a particular area. And not only in the production, but particularly also in the further processing, transfer and transport of plastics microplastics into the environment.

The Darmstadt scientists recently took the first samples from a company producing plastic granulates. Like many large chemical companies, for logistical reasons it is located on a river. Such sites could contribute to the microplastic pollution of bodies of water, for example if surface water enters the river untreated, explains Barkmann's supervisor Professor Markus Engelhart. Thus, in the worst case, the flood of plastic particles that land on the ground, for example during transfer into transport vehicles, ends up directly in the surrounding waters. The EmiStop team will also examine such entry routes.

Concrete recommendations for action can only be made if the burden is analytically determined, emphasizes Professor Susanne Lackner, Head of the Department of Wastewater Management and a partner of EmiStop. The detection of microplastic in water samples has long been a weak point, and the data accordingly weak. For several years, a complex spectroscopic method, Raman microspectroscopy, has been used here. This technique is also used by the Institute for Environmental and Process Engineering at RheinMain University of Applied Sciences in Rüsselsheim, which also participates in EmiStop.

Hajo Bitter, a PhD student in Lackner's group, is refining a method called differential scanning calorimetry. It is well established in the quality assurance of pure plastics but must be adapted to the more complex wastewater samples. First, researchers sieve out particles larger than five millimetres – which are not microplastics – and then they are destroyed by chemical treatment with oxidants that do not attack plastics. Finally, mineral components such as sand are separated through a special suspension technique. The plastic particles thus isolated are heated in a tiny crucible with a given heating rate up to almost 300 degrees Celsius. The device records the heat flows as a function of the temperature, with an empty crucible serving as a reference. Peaks in the diagram, which occur at the melting points of the contained plastics, provide information about the plastic types as well as their concentrations. So far, scientists have measured six common plastics in this way. However, they only use the method to capture plastic particles larger

than ten microns. In addition, because of the tedious sample preparation, the procedure takes up to two weeks.

Significantly faster, but less accurate are procedures that Luisa Barkmann tests for a first estimate: It determines so-called sum parameters, which do not indicate the content of a single substance but a group of related compounds. In environmental analysis,

for example, organic pollutants containing chlorine, bromine or iodine are recorded together as a sum parameter by standard. Companies must measure this value as standard procedure before introducing wastewater into rivers. If it is elevated and if, additionally, there is a particle load, this indicates contamination with the chlorine-containing plastic PVC. "Although this is not an exact

quantification, it does give companies a quick indication of a microplastic load," says Engelhart.

In line with the title of EmiStop, researchers involved not only want to develop detection methods and record entries, but also stop the industrial emissions of microplastics. Project partner EnviroChemie from Roßdorf, less than ten minutes by car from TU Darmstadt, is already testing flocculants that remove microplastics from wastewater. But how effective is the separation process? Is it enough, or are filters more effective? For the evaluation of deposition techniques, PhD student Bitter is developing a model particle test: Magnetic plastic particles are added to wastewater to be purified as a tracer. Their content before and after treatment can be measured with a magnetic scale – and that is more sensitive than with differential scanning calorimetry while, at the same time, being faster because there is no need for lengthy sample preparation. The model particles consist of plastic with enclosed Nano-iron oxide. Their density can be modified so that they can imitate different types of plastic. The Darmstadt-based scientists are developing the particles in cooperation with project partner BS-Partikel from Mainz.

In short: EmiStop travels a long path from microplastic analysis through mass balancing to emissions reduction measures. A clear interest can be identified within the industry, says Engelhart, and emphasizes: "Our aim is not to pillory companies, but provide them with tools to help them respond quickly to unwanted events."

The author is a science journalist and holds a doctorate in Chemistry.

"We want to provide companies with tools to help them respond quickly to unwanted events."

Project EmiStop

The joint project EmiStop is part of the "Plastics in the Environment" initiative of the Federal Ministry of Education and Research (BMBF). EmiStop is the only one out of a total of 18 projects that deals with industrial wastewater. From the beginning of 2018 until the end of 2020, EmiStop will receive funding totalling 1.83 million euros from the BMBF. In addition to TU Darmstadt, RheinMain University of Applied Sciences and EnviroChemie, particle manufacturer BS-Partikel, and consulting firm inter 3 are also participating in EmiStop. Further information: www.emistop.de

The trick with the perfume for insects

In the next few years, a team from TU Darmstadt will produce the pheromones of important pest insects in plants and make them usable for plant protection.

— By Hildegard Kaulen

Anyone who has ever looked after a plant, whether in the field, in the garden or on the window sill, knows how mercilessly pest plants can attack plants. The culprits are quickly identified. Viruses, bacteria, fungi and insects destroy entire crops and benefit from climate change because they spread more in warm summers and suffer less in mild winters. Presently, these pests are mainly fought with pesticides. However, these substances also decimate beneficial insects, reduce biodiversity and pollute the soil and groundwater. Sustainable and environmentally sound solutions are sorely needed.

This is where the European SUSPHIRE project comes in, backed by a consortium from England, Spain, Slovenia and the Federal Republic of Germany. From the German side, three professors of the TU Darmstadt are involved: Heribert Warzecha, Professor of Plant Biotechnology, Andreas Jürgens, Professor of Chemical Plant Ecology, and Alfred Nordmann, Professor of Philosophy. The project has ambitious goals. In the future, moths, mealybugs and the like will no longer be killed by insecticides but prevented from propagating by the unorthodox use of pheromones. Typically, female insects invite males to mate through those sexual attractants, known as pheromones. Warzecha and his colleagues will modify plants by gene transfer in such a way that they also produce pheromones. This will confuse the males in such a way that they will miss the brief window of time for mating and no offspring will be produced.

“Because each species of insect synthesizes its own perfume to prepare for mating, pheromones can be used in a very targeted way to confuse and entice away individual species,” explains Professor Warzecha. “Such a perfume sometimes consists of a single pheromone, sometimes

of several pheromones, but it works only for one species and not for others,” continues the pharmaceutical biologist. Pheromones are currently already used in the form of pheromone traps

or sprays. However, the production of these products is very expensive. That's because their chemical structure is complex. Many syntheses are complicated, and much is technically impossible. Therefore, Warzecha and his colleagues want to establish the production of plant pheromones.

Plants have long been used to produce complex proteins or substances because they are a renewable resource and their cultivation can be adapted to respective conditions. That makes them perfect biofactories.

With the right construction manuals in the genome, they auto-synthesize even the most complicated molecules, requiring only an advantageous site with enough water, sunlight and carbon dioxide. Today, a whole range of technical enzymes are already produced in plants, as well as cosmetics and a drug for a rare disease.

The fact that plants can also produce insect pheromones was already demonstrated several years ago by the Spanish project partners and other working groups. Professor Diego Orzaez and his colleagues

from the University of Valencia introduced the genes for the synthesis of moth pheromones into tobacco. They were able to show that the pheromones thus produced function and attract moths. However, these pheromones are not yet released into the air, but remain in the plant cells. Over time, the group intends to develop solutions. Because the moth males hold the pheromone-producing tobacco plant because of the pheromones for a female, this plant has been given the name “Sexy Plant”. This is a first important prototype. “We know from these results that the concept works in principle,” says Professor Warzecha. “So, we can equip plants to protect themselves from insects, thus giving them relevant agricultural added value.”

Warzecha and his colleagues pursue two fundamental strategies. To begin with, they are concerned with producing insect pheromones or their precursors inexpensively to fill pheromone traps with the isolated substances or use them in sprays. That would significantly reduce the cost of producing such products and make their use significantly more profitable. The long-term goal of the group, however, is to bring the pheromone-producing plants to the field along with the crops. Then,

Information

Department of Biology
Plant Biotechnology and Metabolic
Engineering

Prof. Dr. Heribert Warzecha

E-mail: warzecha@bio.tu-darmstadt.de

<https://bit.ly/2P7nLEY>



Part of the interdisciplinary project team: Andreas Jürgens, Janine Gondolf, Heribert Warzecha (from left).

Photo: Katrin Binner

the pheromones would no longer need to be isolated, but could be released by the plants directly into the environment. However, such applications with genetically modified plants are currently subject to strict regulation. “We will not use feed or food plants for the production of the pheromones, but instead, tobacco, and could even bring the plants to the field in special containers,” says Warzecha. “In the coming years, we will work with the authorities to determine what is possible and what is not. The SUSPHIRE project will also address issues of responsible research and the economic consequences of this work”.

Warzecha and his colleagues are currently also intensively searching for the pheromones of mealy bugs, the citrus mealybug (*Planococcus citri*). These bugs ruin many harvests by covering citrus plants with a waxy substance. However, before Warzecha and his colleagues can produce the pheromones of citrus mealybugs in plants, they must know

the genes so that they can deposit the corresponding building instructions in the plants. “To identify pheromone genes, we will compare all messenger ribonucleic acids produced by fertilized and unfertilized females. In the pool of ribonucleic acids formed by unfertilized females, the blueprint for the pheromones should also be present. We will then transfer the gene with appropriate controls into tobacco plants. Then we must see if enough pheromones are formed and if this happens at the right time and in the right place,” Warzecha continues. He and his colleagues hope to be able to produce a range of pheromones in plants and tailor them for specific applications. The need is great. The world market for insecticides in 2022 should be 17.5 billion euros. The concepts of the consortium are much more environmentally friendly.

The author is a science journalist and holds a doctorate in biology.

Supermaterials out of the microwave

Junior research group leader
Dr. Christina Birkel

Using non-conventional methods, Christina Birkel and her colleagues in the Department of Chemistry of the TU Darmstadt produce metallic ceramics and new materials for the energy supply of the future.

By Uta Neubauer

The microwave oven in the laboratory of Christina Birkel, junior research group leader at the TU Darmstadt, is not only larger and significantly more expensive than the usual household device, but also more powerful and fire and explosion-proof. Birkel had the turntable and its plastic support removed. "That would have melted anyway," she says. The chemist uses the oven for the synthesis of substances that experts call MAX phases. M stands for a transition metal, for example for titanium or vanadium, A for a main group element – usually aluminium – and X for carbon, and more rarely also nitrogen. Thus far, approximately 70 members of this family are known.

"Around the turn of the millennium, research efforts in the field of MAX phases have increased significantly," explains Birkel. No wonder, because the materials are scratch-resistant, high-temperature stable and in many cases oxidation-resistant like a ceramic, but they also conduct electricity and sometimes have extraordinary magnetic properties. They are therefore also referred to as metallic ceramics. Similarly to clay minerals, MAX phases have a lamellar structure of alternating A and M-X-M layers.

While researchers worldwide, especially in the US, investigate the properties and potential applications of MAX phases, Birkel is involved in their synthesis. She has optimized a particularly simple method using microwave heating: The metal and graphite powders are pressed into a dense pellet that is subsequently sealed into an evacuated quartz ampoule. This is then surrounded by granular graphite and placed into the microwave oven. Graphite absorbs the energy of microwave radiation particularly well and ensures that the pellet heats to over 1300 degrees-at such high temperatures, MAX phases form.

But this is not the end of the road for Birkel. Because the MXenes, obtained from MAX phases for the first time in 2011, have an even more promising future than the latter. The name indicates the chemistry in this case: The MXene is a MAX phase without the A layers. These were removed with hydrofluoric acid. Although the procedure requires the utmost caution – hydrofluoric acid is highly corrosive – it does fulfil its purpose perfectly, as shown by the electron microscope: "The layered

structure of MAX phases widens and then looks like a fanned-out book." The individual layers separate partially.

The term MXene with the ending "ene" indicates a certain similarity to graphene, the miracle material

Information

Inorganic solid-state chemistry

Dr. Christina Birkel

Email: birkel@ac.chemie.tu-darmstadt.de

www.chemie.tu-darmstadt.de/nachwuchsgruppe-birkel



consisting of pure carbon layers. Regarding the MXene, a variety of applications from battery materials to water purification are also discussed. Recently, Birkel and her colleagues produced a new MXene. It consists of vanadium-carbon layers and is suitable as a catalyst for the hydrogen evolution reaction in the electrolysis of water, as demonstrated by the group of Ulrike Kramm, assistant professor at TU Darmstadt. Water electrolysis is becoming more and more important because it allows to store excessively generated solar or wind energy in the form of hydrogen.

Hydroxyl groups (oxygen and hydrogen), oxygen and fluorine atoms, which bind to the the surface of the layers during hydrofluoric acid treatment, play an important role in the catalytic activity of the MXene. The Birkel group researchers are currently investigating the exact mechanisms with the aim of optimizing the properties of the MXene. For example, organic molecules could be coupled to the layers via the hydroxyl groups. "Thus, according to the Lego principle, numerous new MXenes are imaginable," explains Birkel. So far, only around 20 MXenes are known. The prospective chemistry professor could not have identified a more expandable area of research.

The author is a science journalist and holds a doctorate in chemistry.

Excellent researcher

Christina Birkel has been a Junior Research Group Leader at TU Darmstadt since 2013 and has been funded since 2017 as part of the TU program Athene Young Investigator. In 2017, she received a € 80,000 Exploration Grant from the Boehringer Ingelheim Foundation.

Recent publications

M. H. Tran et al., Adding a New Member to the MXene Family: Synthesis, Structure and Electrocatalytic Activity for the Hydrogen Evolution Reaction of V4C3Tx, ACS Appl. Energy Mater. 2018, DOI: 10.1021/acsaem.8b00652
C. M. Hamm et al., Structural, magnetic and electrical transport properties of non-conventionally prepared MAX phases V2AlC and (V/Mn)2AlC, Mater. Chem. Front. 2018, 483-490, DOI 10.1039/C7QM00488E