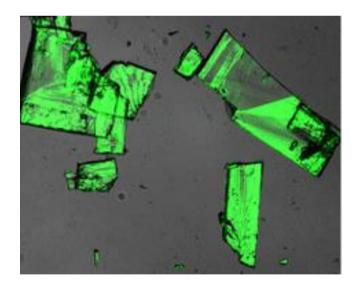


nederlandse vereniging voor kristalgroei

# **FACET**

# **DACG Newsletter**

Newsletter of the Dutch Association for Crystal Growth (DACG), section of the KNCV and the NNV.



FACET Issue 1/2024 April 2024

Editor: Joop H. ter Horst (Info@dacg.nl)



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#### **DACG** board

President: Dr. Carmen Guguta (Technobis)

Secretary: Prof. Dr. Antoine van der Heijden (TUD)

Tresurer: <u>Dr. Hans te Nijenhuis</u> (Malverr

Panalytical)

FACET: Joop H. ter Horst (Tiofarma) Elias Vlieg (Universiteit Nijmegen)

Electable:

Anne Claude (University of Amsterdam)

If you are interested in a role within the DACG just contact us: info@dacg.nl.

## **Cover photo**

SHG microscope images of single crystals of the newly identified conglomerate cocrystal formed from the racemic compound praziquantel and achiral co-former DMTU. The positive SHG signal results in the substrates appearing green and indicates the presence of the noncentrosymmetric structure of the conglomerate cocrystal.

Rapeenun, P.; Gerard, C. J. J.; Pinètre, C.; Cartigny, Y.; Tinnemans, P.; de Gelder, R.; Flood, A. E.; ter Horst, J. H. Searching for Conglomerate Cocrystals of the Racemic Compound Praziquantel. Crystal Growth & Design **2024**, 24 (1), 480–490.

https://doi.org/10.1021/acs.cgd.3c01158.

## From the editor

Dear all,

After the excellent fall symposium at Ardena in Oss, we are scheduled to have the spring symposium at Maastricht University on the 31st of May and organized by the group of Dr Giuditta Perversi. There will also be a PhD student & postdoc early career event the day before the spring symposium. You can register for both via the DACG website (www.dacg.nl). I anyway invite you to have a look at the new website and report to us (info@dacg.nl) whether you like it.

At the fall symposium the DACG committee said goodbye to three members, Marloes Bistervels, Hugo Meekes and Marketta Uusi-Penttilä (many thanks to Marloes, Hugo and Marketta!) and welcomed the new committee members Elias Vlieg and me, Joop ter Horst. Anne Claude is available to be elected in the DACG board by the members in the DACG fall meeting. The board has invited her to already join the board meetings and introduce herself in this FACET, see the next page.

In this issue you will find the report of the fall meeting and more.

Your ideas are welcome, and as always, it is easy to contribute to the FACET. Just send an email with your contribution to the editor via <a href="mailto:info@dacg.nl">info@dacg.nl</a>.

Looking forward to seeing you at the spring symposium!

Joop ter Horst



# Meet the new committee members

## Elias Vlieg

Elias Vlieg, professor in Solid State Chemistry at the Radboud University, Nijmegen. His research group aims to obtain a fundamental understanding of the processes that occur during formation and growth of crystals and to apply this understanding to the prediction and control of crystal properties like perfection and morphology. He recently has been appointed president of the International Organization for Crystal Growth (IOCG), see the previous FACET. The central objective of the IOCG is to establish a platform for scientists in the domain of crystallization, fostering the advancement of both theoretical principles and practical applications within crystal growth, crystal characterization, and interconnected scientific branches.



## Joop ter Horst



After a lifelong presence in academia (Delft University of Technology, University of Strathclyde, University of Rouen) Joop ter Horst last year switched to industry to work in the process industry for Kreber in Vlaardingen. He now starts a new position as Principal Process Scientist at the Dutch pharmaceutical company Tiofarma. He is looking forward to contributing again to the Dutch Association for Crystal Growth, among others by taking care of the association's newsletter FACET.

## **Anne Claude**

My name is Anne, I graduated from a master of chemistry at the Ecole Nationale Supérieure de Chimie de Paris (France) and a master of physics in material science and nano-objects at Sorbonne University (Paris, France). I like working at the interface of these two subjects. I recently started a PhD at the University of Amsterdam where I study hydration/dehydration mechanisms of hydrated salts for thermal energy storage applications. Consecutively, I went to the 2023 Fall Symposium organized by the Dutch Association of Crystal Growth (DACG). I discovered this unique community in the Netherlands of PhDs, post-docs & researchers from academia and industry speaking the language of..."crystals"! This meeting takes place twice a year and is a nice opportunity for everyone in the field to learn new technics, deepen its knowledge and develop its network. Now, I'm very happy to join



the DACG-board as a "Junior Scientist" to bring new ideas to the table so that young generation of researchers could take advantage of this powerful network of renown scientists that is DACG. Looking forward to this new collaboration!



# DACG-NVK Spring Symposium & Early Career Event

We are pleased to join forces with the Dutch Crystallography Society (NVK) for the Spring Symposium on 31 May 2024. The early career event will be hosted on the day before the spring symposium, 30 May 2024. Both events will be organized by the group of Dr Giuditta Perversi at the Faculty of Science and Engineering of Maastricht University.

The DACG-NVK Spring Symposium aims to provide ample opportunity for fruitful discussion and dialogues between experts from different fields of crystallization and to incite collaborations at the international level between the different disciplines on the area of nucleation, crystallization, crystall growth and self-assembly. The DACG & NVK Spring Symposium will feature invited talks by renown researchers from the Netherlands and neighboring countries while it is also possible to contribute talks.

The early career event will be hosted on May 30, focusing on MSc, PhD and post-docs future career opportunities. All participants of the early career gathering are kindly invited to bring a poster about their research. Please send your poster title before April 30, 2024 at info@dacg.nl. We will have two poster sessions dedicated to networking and brainstorming. Please indicate in your registration if you will be taking up this opportunity. The posters will remain in display throughout May 31st. For the participants of the early career event there is a possibility for overnight accommodation (30 to 31 May 2024) in a subsidized Stayokay hostel. This accommodation is subsidized and facilitated by Maastricht University. For more details on accommodation please contact us at info@dacg.nl.

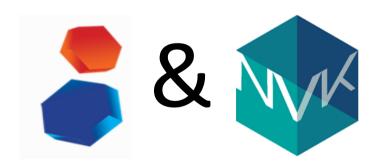
#### Deadline:

15/05/2024 Registration:

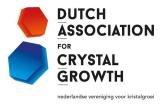
## Registration

The registration fee is €25 for members (DACG, NVK, DGKK, DGK, BGK) and master & PhD students or €40 for non-members. Please make sure you specify your affiliation (DACG, NVK, DGKK, DGK, BGK).

Please register via the dacg website: https://dacg.nl/event/dacg-dcs-spring-symposium/.



Deadline: 31 May 2024



# Piet Bennema Award for Crystal Growth 2024

Every three years the Dutch Association for Crystal Growth DACG distinguishes a young researcher with the Piet Bennema Award for Crystal Growth for his or her high-level scientific research in the field of crystal growth. The prize is intended for the author of the best dissertation or other scientific publications (or a series thereof) that have been processed in an industrial context and are of importance similar to a dissertation. The prize consists of a certificate and a sum of money of € 1000.

#### **Piet Bennema**

Piet Bennema (1932-2016) is one of the founders of the study of crystal growth in the Netherlands. As a professor of chemistry of the solid state from 1976 until his retirement in 1998, he was affiliated with the Radboud University Nijmegen. In this period he elaborated on the theoretical concepts of crystal growth, leading to an improved understanding of the role of the bond strength in the prediction of the morphology of crystals and the role of supersaturation, two-dimensional nucleation, kinetic roughening and spiral growth during crystal growth processes. For his important contributions to the field of crystal growth, he was awarded the Frank Award in 1995 by the International Organization for Crystal Growth.

### **Candidates**

Eligible for the award are both young Dutch and non-Dutch researchers who have largely carried out their research in the scientific field of crystal growth at a Dutch university or a Dutch company.

The candidate must have shown great competence as a researcher as well as scientific originality and productivity. Moreover, it must have a good understanding of the problems of the field.

For candidates who want to be considered on the basis of their dissertation, the latter must have been successfully defended at a Dutch university in the three years prior to the closing of the submission deadline (1 May 2021 - 30 April 2024). For academic publications, it also applies that these must have been published for the most part in the preceding three-year period.

### **Nomination**

Supervisors can nominate candidates by means of a letter of recommendation together with the thesis or other scientific publications, as well as a motivation. The nomination must be submitted in triplicate to the secretary of the DACG.

The submission period for the Piet Bennema Award for Crystal Growth is from 1 October 2023 to 31 May 2024.

#### Award presentation

The Piet Bennema Award for Crystal Growth is awarded by the DACG Board. To this end, the board of the DACG appoints an assessment committee of three experts, who will evaluate the candidates and their scientific work against their competence in the research of crystal growth, scientific quality, productivity and originality and insight into the field.

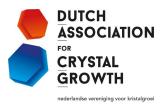
The presentation of the prize and the associated certificate will take place during the autumn meeting of the DACG in October 2024.

On behalf of the board of the DACG,

Antoine van der Heijden

Secretary DACG, Technische Universiteit Delft, Dept. Process & Energy, Leeghwaterstraat 39 2628 CB Delft, antoine.vanderheijden@tno.nl

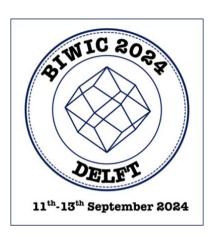
Deadline: 31 May 2024



## **BIWIC 2024**

The 29th BIWIC (International Workshop on Industrial Crystallization) will this year be hosted in Delft by the group of Burak Eral from Delft University of Technology, from September 11 to 13, 2024.

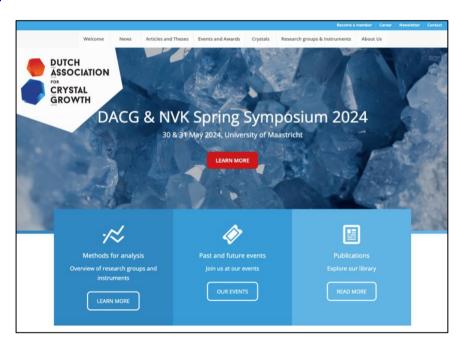
The BIWIC has become an important part of the conference calendar for crystallization groups worldwide. The aim is to gather interested parties from academia, industry, and research institutes to discuss their work and exchange knowledge towards overcoming challenges and advancing the knowledge frontiers in industrial crystallization. It is also a great opportunity to initiate or expand your connections with renowned scientists and industry leaders in the crystallization field in a friendly atmosphere.



Find out more and register on the BIWIC website: www.biwic2024.nl.

# Website

Don't forget to check out our new website (<u>www.dacg.nl</u>) and let us know what you think of it at <u>info@dacg.nl</u>.





# Report DACG fall symposium

## DACG Symposium and General Members Meeting, 30 November 2023

The DACG organized its fall symposium and General Members Meeting on 30 November 2023. Our host was René Steendam from Ardena in Oss. Unfortunately, our chair Carmen Guguta, could not attend the symposium and Hugo Meekes replaced her as chair of the scientific morning and afternoon sessions of this DACG event.

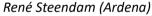
The symposium program consisted of a wide variety of speakers representing the universities of Amsterdam, Leiden, Enschede and Eindhoven as well as several pharmaceutical companies (Ardena, Aspen and Johnson & Johnson).

The first contribution was given by our host **René Steendam**. He presented an overview of the history and current activities and services of Ardena. **Peter van Hoof**, also from Ardena, clearly pointed out to the audience the role and importance of crystallization in the development of pharmaceuticals.



Hugo Meekes (RUN)







Peter van Hoof (Ardena)

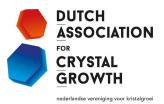
**Rob Geertman** (Janssen Pharmaceutica) took the audience by the hand and navigated us through a jungle of solvates, which are one of the surprises that can be encountered when crystallizing and scaling up pharmaceutical compounds. **Nieké van Gils** (Aspen) explained what Secoya technology can bring in the production of crystals with a desired mean size and size distribution.



Rob Geertman (Janssen Pharmaceutica)



Nieké van Gils (Aspen)



The last presentation of the morning session was given by the PhD student **Michaela Eberbach** (TU/e) on changes in the (de)hydration pathways of CaCl<sub>2</sub> (a material used for energy storage applications) under conditions of nanometer confinement.

After lunch the General Members Meeting of the DACG was held, chaired by Hans te Nijenhuis (replacing Carmen Guguta). Afterwards the scientific part of the symposium continued with a presentation given by **Valent Oldenkotte** (PhD student at Univ Twente) on the 'boring' material VSi<sub>2</sub>, which happened to harbor fascinating physics.





Michaela Eberbach (TU/e)

Valent Oldenkotte (Univ Twente)

Christiaan van Campenhout (PhD student at AMOLF) showed the audience new techniques, inspired by Liesegang rings, to form patterned structures using reaction-diffusion driven crystallization. **Nicolas Magnard** (Univ Leiden) was the final speaker of this fall symposium with a presentation on polymorphism control of manganese oxide nanoparticles (which are a good candidate for effective energy storage and conversion) in hydrothermal synthesis.

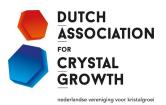




Christiaan van Campenhout (AMOLF)

Nicolas Magnard (Univ Leiden)

A tour along the experimental facilities of Ardena concluded this successful DACG symposium. We were very happy that more than 50 participants attended this DACG event! The DACG would like to thank Ardena, especially René Steendam and Ellis Meerdink, for their excellent hosting of the DACG in Oss! December 2023, Antoine van der Heijden



# A selection of recent publications

Peeters, W. H. J.; Vettori, M.; Fadaly, E. M. T.; Danescu, A.; Mao, C.; Verheijen, M. A.; Bakkers, E. P. A. M. Onset of Uncontrolled Polytypism during the Au-Catalyzed Growth of Wurtzite GaAs Nanowires. *Phys. Rev. Mater.* **2024**, *8* (2), L020401. https://doi.org/10.1103/PhysRevMaterials.8.L020401.

Gerard, C. J. J.; Pinetre, C.; Cercel, H.; Charpentier, M. D.; Sanselme, M.; Couvrat, N.; Brandel, C.; Cartigny, Y.; Dupray, V.; ter Horst, J. H. Phase Diagrams of Praziquantel and Vanillic Acid Cocrystals: Racemic Compound and Conglomerate System. *Crystal Growth & Design* **2024**. https://doi.org/10.1021/acs.cgd.4c00114.

Vries, T. E. de; Vlieg, E.; Gelder, R. de. Unravelling the Structure of the CSD Cocrystal Network Using a Fast Near-Optimal Bipartisation Algorithm for Large Networks. *CrystEngComm* **2024**, *26* (2), 192–202. <a href="https://doi.org/10.1039/D3CE00978E">https://doi.org/10.1039/D3CE00978E</a>.

Le Dizès Castell, R.; Mirzahossein, E.; Grzelka, M.; Jabbari-Farouji, S.; Bonn, D.; Shahidzadeh, N. Visualization of the Sol–Gel Transition in Porous Networks Using Fluorescent Viscosity-Sensitive Probes. *J. Phys. Chem. Lett.* **2024**, *15* (2), 628–635. https://doi.org/10.1021/acs.jpclett.3c02634.

M. H. Bistervels, A. van der Weijden, H. Schoenmaker, M. Kamp, W. L. Noorduin, Compose and Convert: Controlling Shape and Chemical Composition of Self-Organizing Nanocomposites. *Adv. Funct. Mater.* 2024, 2403715. https://doi.org/10.1002/adfm.202403715

Runhua Wang, Zhengshuo Zhan, Bingnan Song, Michel Saakes, Renata D. van der Weijden, Cees J.N. Buisman, Yang Lei, Electrochemical route outperforms chemical struvite precipitation in mitigating heavy metal contamination, Journal of Hazardous Materials, 465, 2024, 133418, ISSN 0304-3894, https://doi.org/10.1016/j.jhazmat.2023.133418.

Melian A.R. Blijlevens, Ekaterina D. Garina, Quirine D.K. Wildeman, Roy van Alst, Natalia Mazur, Hugo Meekes and Elias Vlieg, NaI as suitable alkali halide hydrate for domestic thermochemical heat storage, Journal of Energy Storage, **88** (2024) 111651, 1-12. <a href="https://doi.org/10.1016/j.est.2024.111651">https://doi.org/10.1016/j.est.2024.111651</a>.

Shani, L.; Lueb, P.; Menning, G.; Gupta, M.; Riggert, C.; Littmann, T.; Hackbarth, F.; Rossi, M.; Jung, J.; Badawy, G.; Verheijen, M. A.; Crowell, P. A.; Bakkers, E. P. A. M.; Pribiag, V. S. Diffusive and Ballistic Transport in Thin InSb Nanowire Devices Using a Few-Layer-Graphene-AlOx Gate. *Mater. Quantum. Technol.* **2024**, *4* (1), 015101. https://doi.org/10.1088/2633-4356/ad2d6b.



# **Thesis**

Marco Rossi, Epitaxy of Bottom-Up Grown InSb Nanostructures

PhD defense: 23 mei 2024, Eindhoven University of Technology, Eindhoven

Promoter: prof. dr. Erik Bakkers

Co-promoter: dr. Marcel A. Verheijen

Quantum computers are a revolutionary computing paradigm based on quantum mechanics. They use qubits, the quantum equivalent of bits, to potentially solve problems that classical computers cannot. Preserving the delicate quantum state of qubits is a challenge due to decoherence caused by interactions with the environment. Topological quantum computation offers a promising solution by utilizing Majorana zero modes (MZMs), which are quasiparticles excitations that are resistant to local sources of decoherence. This inherent robustness makes MZMs highly desirable for quantum information processing. Despite various theoretical proposals outlined the necessary conditions for achieving MZMs, experimental realization has yet to be achieved, leaving the existence of MZMs as an open question. The primary impediment to detecting MZMs currently stems from the level of disorder (e.g. crystal defects, impurities, surface roughness) present in the semiconductor-superconductor hybrid devices required for testing their existence. Furthermore, providing definitive proof necessitates the fabrication of a material platform wherein MZMs can be intricately braided within a complex network. These challenges require concerted material science efforts to provide such platform with minimal disorder. This thesis focuses on the bottom-up epitaxy of free-standing nanostructures made of indium antimonide (InSb), a promising semiconductor for constructing such devices due to its unique physical properties.

Lian Blijlevens, Assessing Salt Hydrates For Thermochemical Heat Batteries

PhD defense: 19 December 2023, Radboud Universiteit, Nijmegen

Promotor: Prof. dr. Elias Vlieg Co-promotor: Dr. Hugo Meekes

Everybody wants to have a warm house in the winter, but this should preferably be done without increasing global warming by using fossil fuels. However, currently almost half of domestic heating comes from gas or other fossil fuels so an alternative sustainable source needs to be found. Luckily, the sun produces enough thermal energy, but this is unevenly distributed throughout the year. This gives a mismatch between an excess of solar heat in summer and a shortage in winter. By using a heat battery this mismatch can be mitigated. Thermochemical heat storage in salt hydrates is one of the solutions currently on a pathway to commercialization. Meanwhile, researchers are still working on selecting the best materials and understanding their hydration and dehydration behaviour. This thesis contributes to this research on the material level by evaluating salt hydrates and when promising studying their properties. https://hdl.handle.net/2066/299116.