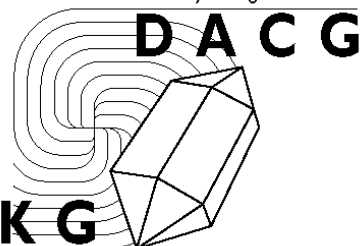


# FACET

dutch association for crystal growth



DACG NEWSLETTER

NVKG

nederlandse vereniging voor kristalgroei

September 2022

Issue 2

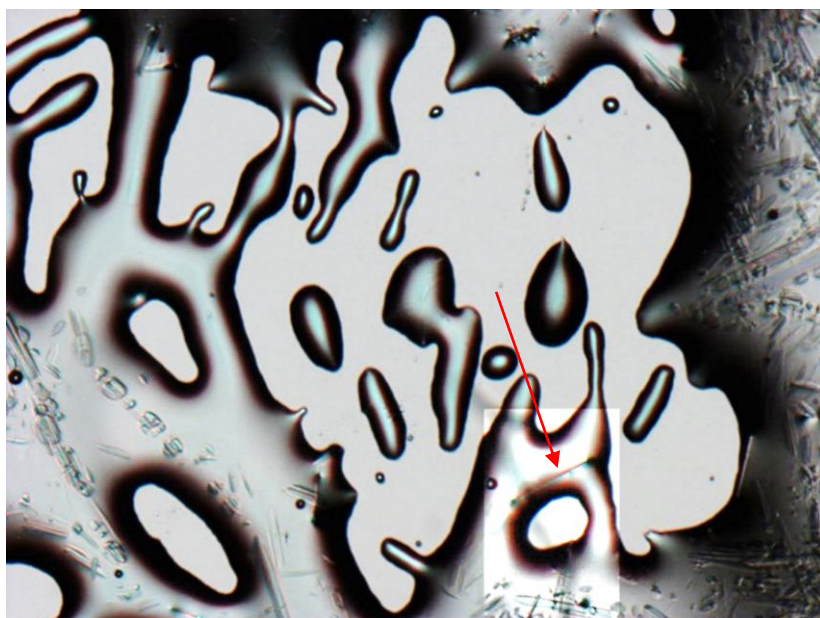
## FACET

Newsletter of the Dutch

Association for Crystal Growth

(DACG), section of the KNCV and

the NNV.



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## DACG Secretary

[Prof.Dr. Antoine van der Heijden](#)

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## DACG board

[Dr. Carmen Guguta](#) (Technobis) president

[Prof.Dr. Antoine van der Heijden](#) (TUD) secretariat

[Dr. Hans te Nijenhuis](#) (Malvern Panalytical) treasurer

[Dr. Hugo Meekes](#) (RU) webmaster

[Dr. Marketta Uusi-Penttilä](#) (Aspen Oss) FACET

## Cover figure

Hot-stage microscopy image of gradually melting monohydrate crystals and the arrow indicating the appearance of the first thin needle-shaped anhydrate crystal (Aspen Oss internship of Tobian de Ruiter, Faculty FNWI, Radboud University, Nijmegen).

## From the editor

Dear all,

I hope that you have had a relaxing summer.

Technobis is hosting the annual meeting 2022 and fall symposium at Technobis on Friday October 21<sup>st</sup>.

Related to our 50th anniversary, check NTVN for two papers on physics-related aspects of crystal growth. *“Linksom of rechtsom met kristallen”* Hugo Meekes and Elias Vlieg appeared in the September issue. Wim Noorduin’s paper will be published in the October issue.

Due to postponement of several conferences and symposia, our 50<sup>th</sup> anniversary will take place in 2023 (50+1 years). Please do not hesitate to share your highlights of 50 years of crystal growth in the Netherlands, including pictures of your historical crystal growth or crystallization installations.

Your ideas are welcome, and as always, it is easy to contribute to the FACET. Just send an email to the editor: [Marketta Uusi-Penttilä](#)

Keep safe!

*Marketta Uusi-Penttilä*

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# Save the date - 20-22 March 2023!

International conference celebrating the 50th anniversary of the DACG in Amsterdam.

More information will follow on the DACG website.

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# DACG Spring Symposium 2022

25 May 2022, AMOLF, Amsterdam

On 25 May, 2022, the DACG organized its spring meeting hosted at AMOLF, Amsterdam. The local organizers were Wim Noorduin and Marloes Bistervels. This was the first 'live' meeting after two years of COVID19 during which several symposia had to be either cancelled or organized online. Traditionally the spring meeting is primarily intended to give the floor to PhD students to present their (intermediate) results as a preparation for presenting their research for a larger audience, e.g. at international conferences. During this symposium also the KNCV Piet Bennema Crystal Growth Award 2021 ceremony was scheduled. This was originally planned for the symposium in October last year, but since this was an online symposium, it was decided to postpone the ceremony to this spring meeting.



From left to right: **Wim Noorduin**, **Carmen Guguta** and **Marloes Bistervels**

After the opening of the symposium by Carmen Guguta (DACG-chair) and Wim Noorduin (AMOLF), the first lecture was given by Marloes Bistervels (AMOLF) presenting her results on light-directed crystallization: by using UV-light she managed to control the formation of nanocomposites very precisely. After this opening lecture, Sevgi Polat (TU Delft) presented results from her PhD research on the effect of hyaluronic acid on the structure and morphology of calcium oxalate crystals. Rozeline Wijnhorst (University of Amsterdam) gave a presentation on 'floppy' hydrated salt crystals: microcrystals of natural inorganic salt hydrates lose their facets and become soft and deformable when in contact with their saturated salt solution at their deliquescence point.



**Marloes Bistervels** (AMOLF): *Light-directed crystallization*



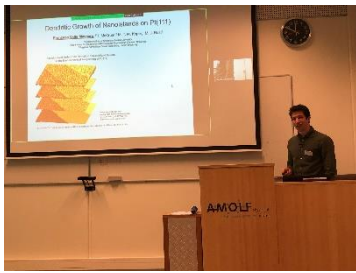
**Sevgi Polat** (TU Delft): *Elucidating the effect of hyaluronic acid on the structure and morphology of calcium oxalate crystals*



**Rozeline Wijnhorst** (University of Amsterdam): *'Floppy' hydrated salt crystals*

Just before lunch, a speed-dating session was organized by Marloes Bistervels. Participants were divided into groups consisting of a mix of people working either at academia, research institutes or industry. Within each group people could shortly introduce themselves and answer each other's questions. The speed-dating event was an informal way to get to know new people in the field of crystallization, in this way lowering the threshold to contact people you do not (yet) know. During lunch there was the possibility to have a look at the posters

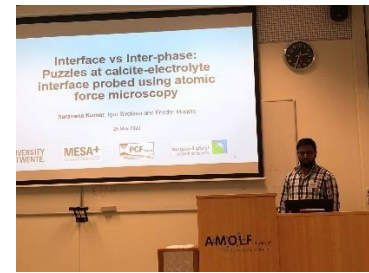
and discuss the content with the presenting PhD students.



**Francesc Valls Mascaro** (Leiden Univ):  
*Dendritic growth of nanoislands on Pt(111)*



**Sergej Seepma** (Utrecht Univ):  
 $\{Ba^{2+}\};\{SO_4^{2-}\}$  of  $BaSO_4$  crystal nucleation and growth in aqueous solutions: a dynamic light scattering study



**Saravana Kumar** (Univ of Twente):  
*Probing the dynamic nature of calcite-electrolyte interface using atomic force microscopy*

After many years, we were able to revive the contacts with the geochemistry group at the University of Utrecht and Sergej Seepma presented his results on the asymmetrical dependence on  $\{Ba^{2+}\};\{SO_4^{2-}\}$  of  $BaSO_4$  crystal nucleation and growth in aqueous solutions using dynamic light scattering. Saravana Kumar (University of Twente) shared his results on the dynamic nature of calcite-electrolyte interface probed with atomic force microscopy.

After the last presentation from the regular symposium programme, the KNCV Piet Bennema Crystal Growth Award 2021 was handed out by Rob Geertman (member of the jury) to Ricardo Cunha for his PhD research performed at the Wageningen University & Research (WUR) on “*Anaerobic calcium phosphate granulation*”. The jury, consisting of Dominique Maes (chair), Rob Geertman and Paul Poedt, selected the PhD thesis of Ricardo Cunha from three nominated PhD theses. One of the two other nominated candidates, Sander Brugman (PhD thesis “*The structure of mineral-electrolyte interfaces*”, Radboud University Nijmegen), was presented a certificate of honorable mention. The third nominated candidate, Hans Hendrikse (PhD thesis “*On the conversion of nanocomposite architectures*”, AMOLF), could not attend the symposium and his certificate has been handed over later on. After the award ceremony, Ricardo closed the symposium with his lecture, presenting the results of his award winning PhD research.



**Sander Brugman** (Radboud University Nijmegen)



**Ricardo Cunha** (Institute of Energy and Environmental Technology, Duisburg, Germany) was handed over the KNCV Piet Bennema Crystal Growth Award 2021 by **Rob Geertman** (left)

The DACG symposium was attended by 45 participants. On behalf of the DACG board, we would like to acknowledge Wim Noorduyn and Marloes Bistervels and their supporting staff Erny Lammers, Teresa van der Linden and Puck Beekman, for organizing this successful symposium and for hosting the DACG community at AMOLF.

*Antoine van der Heijden*





## DACG Annual meeting 2022 & Fall Symposium

*Technobis, Alkmaar, 21 October 2022*

09:30 – 10:00	<b>Registration and coffee</b>
10:00 – 10:15	<b>Welcome and introduction</b> Carmen Guguta
10:15 – 10:40	<b>Effect of solvent composition on solubility, thermodynamics, MSZW and crystal habit of ascorbic acid</b> Jyoti Yadav (Technobis)
10:40 – 11:05	<b>Artificial neural networks for co-crystal prediction</b> Elias Vlieg (Radboud University Nijmegen)
11:05 – 11:50	<b>TBA</b> Peter Daudey (Delft University of Technology)
11:50 – 12:15	<b>Size and microstructure control in crystallization from deep-eutectic solvents</b> Giuditta Perversi (Maastricht University)
12:15 – 12:45	<b>Lunch</b>
12:45 – 13:45	<b>Annual meeting DACG / poster session</b>
13:45 – 14:30	<b>Company visit</b>
14:30 – 14:55	<b>The impact of solution stoichiometry on the nucleation and growth of calcium carbonate</b> Mariëtte Wolthers (Utrecht University)
14:55 – 15:20	<b>Solid form screening enhanced by advanced tools for characterization of pharmaceutical compounds</b> Mihaele Pop (TeraCrystal)
15:20 – 15:50	<b>Coffee break</b>
15:50 – 16:15	<b>Screening double salt sulfate hydrates for application in thermochemical heat storage</b> Wessel Kooijman (Radboud University Nijmegen)
16:15 – 16:40	<b>Non-random island nucleation in the electrochemical roughening on Pt(111)</b> Marcel Rost (Leiden University)
16:40 – 17:30	<b>Drinks / nibbles</b>

**Venue:** Technobis, Pyrietstraat 2, 1812 SC Alkmaar

### Registration

Please register through [DACG Autumn Symposium - Crystallization Systems](#)  
**by 14 October 2022.**

## DACG Annual Meeting 2022

*21 October 2021 12:45-13:45, Technobis, Alkmaar*

1. Opening
2. Finalize agenda
3. Minutes Annual meeting 8 October 2021 (online)
4. Documents sent / received: report of the financial audit committee (see agenda item 6)
5. Annual Report Oct 2021 – Oct 2022
6. Financial
  - (a) Annual Financial Report Oct 2021 – Sep 2022
  - (b) Report Financial Audit Committee
  - (c) Budget 2022-2023
7. Board

Role	2021 – 2022	Appointment deadline
President	Carmen Guguta	Step down Oct 2024
Secretariat	Antoine van der Heijden	Step down Oct 2022 (re-electable)
Treasurer	Hans te Nijenhuis	Step down Oct 2024
Webmaster	Hugo Meekes	Step down Oct 2023
FACET	Marketta Uusi-Penttilä	Step down Oct 2023

In 2021 Marloes Bistervels (PhD student AMOLF) started to support the board as a representative of the Young-DACG.

Antoine van der Heijden steps down, but is re-electable. DACG-members who would like to apply for a board membership, can announce themselves by sending an e-mail to the DACG secretariat ([a.e.d.m.vanderheijden@tudelft.nl](mailto:a.e.d.m.vanderheijden@tudelft.nl)), ultimately by 14 October 2022.

8. 2023: DACG 50 years (update by Elias Vlieg)
10. Status Stichting
11. Young-DACG (update by Marloes Bistervels)
12. Activities 2022 – 2023
  - a. KNCV-event “Avond van de Chemie”, 13 October 2022, De Leidse Schouwburg, Leiden (<https://www.kncv.nl/bijeenkomsten/1051/avond-van-de-chemie-2022#YxNmTchBzIU>)
  - b. NNV Advisory Board Meeting, December 2022 (section boards will be invited)
  - c. 20-22 March 2023: international conference celebrating the 50th anniversary of the DACG, Amsterdam
  - d. October 2023: DACG annual meeting + symposium, location/date to be decided
13. Questions before closure of meeting
14. Adjourn



## Annual Report Dutch Association for Crystal Growth (DACG) October 2021 –September 2022

### Secretariat

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 2628 CB Delft  
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 E-mail: [a.e.d.m.vanderheijden@tudelft.nl](mailto:a.e.d.m.vanderheijden@tudelft.nl)  
 Web: [www.dacg.nl](http://www.dacg.nl)

### Members

The total number of regular members is 58, of which 7 are lifetime member. Furthermore we had had an additional number of 10 “calendar year” members. The “calendar year” members registered in 2021-2022 during the spring symposium held on 25 May 2022, are offered the possibility to attend a DACG symposium for the registration fee of a regular DACG member for the “live” symposium to be organized in October 2022.

### Board

The DACG Board is shown in the table below. The Board had seven online video meetings and one face-to-face meeting (25 March 2022) at Radboud University Nijmegen. At the annual meeting in October 2021, Pieter Vonk (treasurer) and Hans te Nijenhuis (president) stepped down from the board. Carmen Guguta was elected to the board and Hans was re-elected. At the first board meeting after the annual meeting Carmen was appointed as the new president of the DACG and Hans took over from Pieter as the treasurer. In 2021 Marloes Bistervels (PhD student AMOLF) started to support the board as a representative of the Young-DACG.

Role	2021 – 2022	Appointment dead-line	E-mail
President	Carmen Guguta	Step down Oct 2024	carmen.guguta@technobis.com
Secretary	Antoine van der Heijden	Step down Oct 2022	a.e.d.m.vanderheijden@tudelft.nl
Treasurer	Hans te Nijenhuis	Step down Oct 2024	hans.te.nijenhuis@panalytical.com
Webmaster	Hugo Meekes	Step down Oct 2023	h.meekes@science.ru.nl
FACET	Marketta Uusi-Penttilä	Step down Oct 2023	muusipenttila@nl.aspenpharma.com

### FACET Newsletter

The DACG Newsletter, FACET, was issued in April and September 2022. Marketta Uusi-Penttilä is the editor of the FACET. The objective of the newsletter is to stimulate the communication between scientists and users in the area of crystallization in the Netherlands. The newsletter publishes summaries of relevant PhD theses, upcoming events related to crystallization (conferences, symposia), highlights in crystal growth research and other activities relevant to crystal growers. Several academic scientists have been requested to collect news from their network/colleagues as input to the newsletter, but also members may submit input. Furthermore, initiatives, decisions and plans of the DACG will be published in the FACET Newsletter. FACET is issued electronically or can be downloaded from the DACG website. An overview of the DACG correspondents can be found on the DACG website.

## UBO

UBOs (Ultimate Beneficial Owners) are the ultimate beneficiaries of an organization, in other words, the persons in charge. The UBOs of the DACG are its board members and these have been officially registered at the KvK (Chamber of Commerce in the Netherlands).

## Stichting “International Conferences on Crystal Growth”

Currently the Stichting Board consists of the DACG Board members. The modifications in the board have been registered at the KvK. Also the UBOs of the Stichting have been officially registered at the KvK.

## Website

The DACG website ([www.dacg.nl](http://www.dacg.nl), hosted by Radboud University Nijmegen) provides information regarding the structure and activities of the association. All issues of the FACET Newsletter since 2000 are available electronically; links to Dutch research groups in the area of crystallization are available as well as those of foreign DACG ‘sister’ associations. We welcome any suggestions for improvements; please contact Hugo Meekes ([h.meekes@science.ru.nl](mailto:h.meekes@science.ru.nl)).

This year Carmen Guguta approached several companies for designing a new logo and building a new website. Progress will be presented at the Annual Meeting planned to be held in October 2022.

## KNCV Piet Bennema Crystal Growth Award 2021

Last year a jury (consisting of Prof Dominique Maes (Vrije Universiteit Brussel, chair), dr Rob Geertman (Janssen Pharmaceutica) and dr Paul Poodt (TNO)) selected dr Jorge Ricardo Cunha<sup>1</sup> (WUR) as the winner of the 2021 award. The award ceremony was originally planned for the symposium in October 2021, but due to the COVID19 measures, this symposium was held online. The award ceremony was therefore postponed to the spring symposium held on 25 May 2022 at AMOLF, where the award was handed out to Ricardo Cunha by Rob Geertman. The other two nominated scientists, dr Sander Brugman<sup>2</sup> (Radboud University, also present at the symposium) and dr Hans Hendrikse (AMOLF) received a certificate with an honorable mention.

## Young-DACG

The initiatives to make the DACG also an attractive platform for young researchers are managed by Marloes Bistervels (AMOLF). As a result of the inventory survey and focus session, it was decided to set up a telegram group. Every DACG member (industry and academia) can join the group. It has the intention to function as a quick communication channel, where informally help and advice can be asked, but also where updates of events or field-related announcements can be presented. The size and activity of the group are still low but can grow over time when the group is promoted at DACG events. A speed-date activity was organized during the first “live” event after two years (25 May 2022). Groups with mixed professions were made to discuss crystal-growth-related topics, which encouraged the integration of the different fields. The LinkedIn group is not yet launched, this is decided to go together with the new website.

## Meetings / excursions organized by DACG

On October 8, 2021 the DACG’s symposium and annual meeting was organized online (due to the COVID19 measures). On May 25, 2022 the DACG organized their Spring Meeting hosted at AMOLF, the first “live” event after two years. During the symposium the KNCV Piet Bennema Crystal Growth Award 2021 was officially handed out to Ricardo Cunha.

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<sup>1</sup> Now affiliated with the Institut für Energie- und Umwelttechnik E.V. (IUTA), Duisburg, Germany.

<sup>2</sup> Now affiliated with Symeres, Weert, The Netherlands.

### Activities relevant to DACG community

On 8 December 2021 Hans te Nijenhuis attended the online NNV Advisory Board Meeting on behalf of the DACG Board.

### DACG's 50<sup>th</sup> anniversary

In 1972 the Kontaktgroep Kristalgroei Nederland (KKN) was established. In 1998, the name was changed in Nederlandse Vereniging voor Kristalgroei, NVKG / Dutch Association for Crystal Growth, DACG. This implies that in 2022 the DACG celebrates its 50<sup>th</sup> anniversary. A commission, led by Prof Elias Vlieg, has been founded in 2019 that has started the preparations for organizing an international symposium similar to the BRIDGE symposium held in the past. The previously communicated date for this event (23-25 March 2022) was abandoned due to the fact that several other international crystal growth conferences were postponed to 2022 due to COVID19. The DACG board decided to postpone the 50<sup>th</sup> anniversary to 2023, in order to prevent too much interference with the other international meetings. Next to NL, UK and Germany, we also intend to invite our Belgian, French and Irish colleagues. The international symposium is planned to be organized in Amsterdam on 20-22 March 2023.

Furthermore, the DACG board is looking for other possibilities to celebrate half a century of crystal growth in the Netherlands. In close cooperation with the editorial board of the *Nederlands Tijdschrift voor Natuurkunde (NTvN)*, two papers were published on physics-related aspects of crystal growth, one authored by Hugo Meekes and Elias Vlieg on "*Linksom of rechtsom met kristallen*" (appeared in NTvN September 2022, including an editorial about the 50<sup>th</sup> anniversary of the DACG by Hans te Nijenhuis) and another one by Wim Noorduin (scheduled for one of the next issues of the NTvN in 2022). DACG members who would like to share their ideas or support the DACG board with the organization of the 50<sup>th</sup> anniversary of the DACG are most welcome. Please contact the secretary.

### Upcoming activities

- 13 October 2022: KNCV-event "Avond van de Chemie", De Leidse Schouwburg, Leiden; more information can be found on the KNCV website:  
<https://www.kncv.nl/bijeenkomsten/1051/avond-van-de-chemie-2022#.YxNmTchBzIU>
- December 2022: NNV Advisory Board Meeting (section boards will be invited)
- 20-22 March 2023: international conference celebrating the 50<sup>th</sup> anniversary of the DACG, Amsterdam
- October 2023: DACG Fall Meeting; date/location to be decided



## Recent publications

- W. Kooijman, D.J. Kok, M.A.R. Blijlevens, H. Meekes, E. Vlieg, Screening double salt sulfate hydrates for application in thermochemical heat storage, *Journal of Energy Storage*, **55** (2022) 111770.

### Affiliation

- Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands

In this paper a relatively new class of thermochemical compounds is tested for their heat storage potential. 24 different double salt sulfate hydrates with the general formula  $A^I_2B^{II}(SO_4)_2 \cdot nH_2O$  were synthesized and screened for the desirable properties of a thermochemical heat battery material. The materials were tested on the following set of criteria: energy density  $\geq 1.3 \text{ GJ/m}^3$ , dehydration temperature  $\leq 120 \text{ }^\circ\text{C}$ , 10-fold cyclability at  $P_{H_2O} \leq 12 \text{ mbar}$ . The 24 salts have dehydration temperatures between 55 and 198  $^\circ\text{C}$  and energy densities between 1.1 and 2.0  $\text{GJ/m}^3$ .  $(NH_4)_2Zn(SO_4)_2 \cdot 6H_2O$  is the only material that passes all the set criteria and is therefore suitable for further investigation. This material has an energy density of 1.78  $\text{GJ/m}^3$ , a dehydration temperature of 84  $^\circ\text{C}$  after one dehydration-hydration cycle and can perform at least 10 cycles without loss of performance. There are five other salts of interest that meet two out of the three criteria.  $(NH_4)_2Ni(SO_4)_2 \cdot 6H_2O$  has a 1.8  $\text{GJ/m}^3$  energy density and is cyclable 10 times, but has a dehydration temperature of 132  $^\circ\text{C}$ .  $(NH_4)_2Fe(SO_4)_2 \cdot 6H_2O$ ,  $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ ,  $Cs_2Mg(SO_4)_2 \cdot 6H_2O$  and  $Cs_2Ni(SO_4)_2 \cdot 6H_2O$  have energy densities of 1.6 to 1.76  $\text{GJ/m}^3$  and dehydration temperatures below 120  $^\circ\text{C}$ , but they require 22.7 mbar to achieve cyclability.

- T. Lerdwiriyanupap, G. Belletti, P. Tinnemans, R. Cedeno, H. Meekes, E. Vlieg, A. Flood, The influence of Ostwald's rule of stages in the deracemization of a compound using a racemic resolving agent, *Cryst. Growth Des.*, **22** (2022), 1459–1466.

### Affiliations

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The stereoisomeric system of rac-2-phenylglycinamide (PGA) and rac-N-acetyl tryptophan (NAT) is significant in the application of chiral resolution because it has been shown that this system can be used for enantioseparation of PGA and/or NAT using a novel deracemization route of the conglomerate salt formed. However, it was also found that the conglomerate salt eventually converted into different crystal forms that limited the time available for the separation. Herein, we try to understand the phase conversion occurring in this system using DSC, PXRD, and SC-XRD. The related structures of the salt (two polymorphs of the more stable homochiral (dd- and ll-) salts and one polymorph of the less stable heterochiral (dl- and ld-) monohydrate salts) are demonstrated and discussed relating to their relative stabilities. The successful deracemization was demonstrated using the heterochiral (dl- or ld-) monohydrate salts. However, following Ostwald's rule of stages, only limited time is available for the deracemization before the metastable compound converts into the more stable homochiral (dd- and ll-) pair. Moreover, the occurrence of the (dd- and ll-) phase always coincides with the formation of yet another phase of the racemic compound containing four components in a crystal. Ostwald's rule of stages here thus involves three steps and phases and is highly significant during the deracemization of the homochiral species.

- M.A.R. Blijlevens, N. Mazur, W. Kooijman, H. Fischer, H. Huinink, H. Meekes, E. Vlieg, [A study of the hydration and dehydration transitions of SrCl<sub>2</sub> hydrates for use in heat storage](#), *Solar Energy Materials and Solar Cells*, **242** (2022) 111770.

#### Affiliations

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- Technical University Eindhoven, P.O. Box 513, Department of Applied Physics, 5600, MB, Eindhoven, the Netherlands
- Netherlands Organization for Applied Scientific Research (TNO), High Tech Campus 25, 5656, AE, Eindhoven, the Netherlands

We have experimentally determined the main thermodynamic properties of SrCl<sub>2</sub>, a potentially promising salt for thermochemical heat storage. We found a high energy density of  $2.4 \pm 0.1$  GJ/m<sup>3</sup> and proved full cyclability for at least 10 cycles going from the anhydrate to the hexahydrate without chemical degradation. We have experimentally determined the thermodynamic equilibria for each individual transition and the corresponding metastable zones. We find that the metastable zone is widest for the anhydrate to monohydrate transition and decreases with each subsequent hydration step. We have also established that the observed nucleation kinetics are highly dependent on the preparation of the sample. Depending on the preparation conditions, some seeds of the precursor phase can remain in the sample thereby influencing the induction times for the transition. In heat storage applications we recommend selecting conditions well away from the phase transition lines (at least outside the metastable zone) and to leave some seeds of the phase to be transferred in order to increase the transition speed.

- S.J.T. Brugman, P. Accordini, F. Megens, J.J. De vogelaer, E. Vlieg, [Ordered and disordered carboxylic acid monolayers on calcite \(104\) and muscovite \(001\) surfaces](#), *J. Phys. Chem. C*, **126** (2022) 8855-8862.

#### Affiliations

- Solar Technologies and Applications, TNO/Solliance, Eindhoven, The Netherlands
- Applied Materials Science, Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands
- Solid State Chemistry, Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The adsorption of carboxylic acid molecules at the calcite (104) and the muscovite (001) surface was investigated using surface X-ray diffraction. All four investigated carboxylic acid molecules, hexanoic acid, octanoic acid, lauric acid, and stearic acid, were found to adsorb at the calcite surface. Whereas the shortest two carboxylic acid molecules, hexanoic acid and octanoic acid, showed limited ordering and a flexible, disordered chain, the two longest carboxylic acid molecules form fully ordered monolayers, i.e., these form highly structured self-assembled monolayers. The latter molecules are oriented almost fully upright, with a tilt of up to 10°. The oxygen atoms of the organic molecules are found at similar positions to those of water molecules at the calcite–water interface. This suggests that in both cases, the oxygen atoms compensate for the broken bonds at the calcite surface. Under the same experimental conditions, stearic acid does not adsorb to K<sup>+</sup> and Ca<sup>2+</sup>-functionalized muscovite mica because the neutral molecules do not engage in the ionic bonds typical for the mica interface. These differences in adsorption behavior are characteristic for the differences of the oil–solid interactions in carbonate and sandstone reservoirs.

- M. van Eerden, J. van Gastel, G.J. Bauhuis, E. Vlieg, J. Schermer, Comprehensive analysis of photon dynamics in thin-film GaAs solar cells with planar and textured rear mirrors, *Solar Energy Materials and Solar Cells*, **242** (2022) 111770.

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This study describes a comprehensive analysis of light trapping and photon recycling (PR) in thin-film GaAs solar cells, explicitly considering the effects of (non-perfect) light scattering at a textured rear mirror. We calculate the probabilities of escape, reabsorption in the absorber and parasitic absorption for internally generated photons, as well as the reflectance, absorptance and parasitic absorptance of externally incident photons. Combined with the internal luminescent efficiency to account for non-radiative recombination non-explicitly, but in a phenomenological manner, device performance metrics such as the short-circuit current density ( $J_{sc}$ ), open-circuit voltage ( $V_{oc}$ ) and its radiative limit, the external luminescent efficiency, the contribution of PR to the  $V_{oc}$  and the power conversion efficiency ( $PCE$ ) are derived. We analyze a typical thin-film GaAs solar cell architecture, consisting of an n-GaAs/p-InGaP heterojunction structure cladded by commonly employed front- and rear-side layer stacks. The probabilities of escape, reabsorption and parasitic absorption and the resulting performance metrics are presented as a function of absorber thickness, rear-mirror reflectivity, haze factor, internal luminescent efficiency, front grid coverage and band tailing. The simulations show that the implementation of a textured rear mirror reduces PR and its importance for device performance. In these textured cells, a high rear-mirror reflectivity and, thereby, efficient PR, is less crucial to achieve  $V_{oc}$  values close to the radiative limit. The increased  $J_{sc}$  in textured cells renders light trapping favorable for the  $PCE$ , regardless of absorber thickness and material quality and despite reduced PR. Furthermore, the impact of an absorbing front grid and lateral transport of internal luminescence on PR is estimated, emphasizing the importance of transparent (non-absorbing) contact layers, at the rear, but importantly, also at the front of the device. To conclude,  $PCE$  limits of 300-nm-thick GaAs solar cells are deduced in the context of an experimentally realized light-trapping scheme based on a randomly textured rear mirror.  $PCE$ s exceeding 25.5% are deemed realistic.

- S. E. Lepinay, R. Nijveld, K.P. Velikov, N. Shahidzadeh, NaCl Crystals as Carriers for Micronutrient Delivery, *ACS Omega*, **7** (2022), No. 33, 28955–28961.

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Iron deficiency leading to anemia is one of the most severe and important nutritional deficiencies in the world today. To combat this deficiency, the fortification of food products with iron is a natural way to increase the global iron uptake. Here, we report a novel strategy for iron encapsulation in NaCl crystals via microscopic inclusions containing dissolved iron salt. The liquid inclusions embedded in the crystal insulate the reactive iron salts from their environment while assuring that iron is in a soluble and bioavailable form. While the size distribution of inclusions remains independent of the evaporation conditions, their density increases during crystallization at lower relative humidity. Using Raman confocal microspectroscopy, we have been able to analyze the morphology, length/thickness ratio, of inclusions and show that inclusions evolve toward a plate-like structure with the increase in size. By growing a pure NaCl shell around the iron-containing NaCl crystals, the stability of the composite crystals can be even further enhanced. The role of halite crystals as a carrier for iron fortification opens the way for the delivery of other types of micronutrients by including them in table salt.

- L. Jacobse, V. Vonk, I.T. McCrum, C. Seitz, M.T.M. Koper, M.J. Rost, A. Stierle, Electrochemical oxidation of Pt(111) beyond the place-exchange model, *Electrochimica Acta*, **407** (2022) 139881

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Oxide formation plays an important role in the degradation of Pt electrocatalysts. However, the exact oxide structure and reaction mechanism are not fully understood. Here, we used in situ surface X-ray diffraction experiments to resolve the oxide formation at a Pt(111) model electrode at potentials near the onset of the oxygen evolution reaction. Fast experiments are possible by using X-ray photons with a high kinetic energy in combination with a large 2D detector. By employing very low potential sweep rates we obtain a more ordered oxidized surface compared to literature data from potential step experiments. This demonstrates that the oxidation process is strongly governed by the reaction kinetics. The increased surface order enables us to disentangle two subsequent oxidation processes; initially the place-exchange process, followed by the formation of a partially disordered oxide in which still 50% of the surface atoms reside on sites commensurate to the Pt(111) surface. The reduction experiments indicate that the place exchange process is structurally reversible, whereas the disordered oxide causes the surface roughening observed during potential cycling. Despite the increased surface order, oxide superstructures are not observed. These results provide important insights in the oxidation and degradation process of Pt(111), which are valuable for the design of improved electrocatalysts and they rationalize operating procedures.



- L. Vincent, E.M.T. Fadaly, C. Renard, W.H.J. Peeters, M. Vettori, F. Panciera, D. Bouchier, E.P.A.M. Bakkers, M.A. Verheijen, Growth-Related Formation Mechanism of I<sub>3</sub>-Type Basal Stacking Fault in Epitaxially Grown Hexagonal Ge-2H, *Advanced Materials Interfaces*, **9** (2022), No. 16, 2102340.

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The hexagonal-2H crystal phase of Ge has recently emerged as a promising direct bandgap semiconductor in the mid-infrared range providing new prospects of additional opto-electronic functionalities of group-IV semiconductors (Ge and SiGe). The controlled synthesis of such hexagonal-2H Ge phase is a challenge that can be overcome by using wurtzite GaAs nanowires as a template. However, depending on growth conditions, unusual basal stacking faults (BSFs) of I<sub>3</sub>-type are formed in the metastable 2H structure. The growth of such core/shell heterostructures is observed in situ and in real time by means of environmental transmission electron microscopy using chemical vapor deposition. The observations provide the first direct evidence of a step-flow growth of Ge-2H epilayers and reveal the growth-related formation of I<sub>3</sub>-BSFs during unstable growth. Their formation conditions are dynamically investigated. Through these in situ observations, a scenario can be proposed for the nucleation of I<sub>3</sub>-type BSFs that is likely valid for any metastable hexagonal 2H or wurtzite structures grown on m-plane substrates. Conditions are identified to avoid their formation for perfect crystalline synthesis of SiGe-2H.

- J.J.P.M. Schulpen, M.A. Verheijen, W.M.M. Kessels, V. Vandalon, A.A. Bol, Controlling transition metal atomic ordering in two-dimensional Mo<sub>1-x</sub>W<sub>x</sub>S<sub>2</sub> alloys, **9** (2022), No. 2, 025016

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The unique optical and electronic properties of two-dimensional transition metal dichalcogenides (2D TMDs) make them promising materials for applications in (opto-)electronics, catalysis and more. Specifically, alloys of 2D TMDs have broad potential applications owing to their composition-controlled properties. Several important challenges remain regarding controllable and scalable fabrication of these alloys, such as achieving control over their atomic ordering (i.e. clustering or random mixing of the transition metal atoms within the 2D layers). In this work, atomic layer deposition is used to synthesize the TMD alloy Mo<sub>1-x</sub>W<sub>x</sub>S<sub>2</sub> with excellent composition control along the complete composition range  $0 \leq x \leq 1$ . Importantly, this composition control allows us to control the atomic ordering of the alloy from well-mixed to clustered while keeping the alloy composition fixed, as is confirmed directly through atomic-resolution high-angle annular dark-field scanning transmission electron microscopy imaging. The control over atomic ordering leads to tuning of the bandgap, as is demonstrated using optical transmission spectroscopy. The relation between this tuning of the electronic structure and the atomic ordering of the alloy was further confirmed through *ab-initio* calculations. Furthermore, as the atomic ordering modulates from clustered to well-mixed, the typical MoS<sub>2</sub> and WS<sub>2</sub> A<sub>1g</sub> vibrational modes converge. Our results demonstrate that atomic ordering is an important parameter that can be tuned experimentally to finely tune the fundamental properties of 2D TMD alloys for specific applications.

- G. Badawy, B. Zhang, T. Rauch, J. Momand, S. Koelling, J. Jung, S. Gazibegovic, O. Moutanabbir, B.J. Kooi, S. Botti, M.A. Verheijen, S.M. Frolov, E.P.A.M. Bakkers, Electronic Structure and Epitaxy of CdTe Shells on InSb Nanowires, *Advanced Science*, **9**, (2022), No. 12, 2105722

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Indium antimonide (InSb) nanowires are used as building blocks for quantum devices because of their unique properties, that is, strong spin-orbit interaction and large Landé  $g$ -factor. Integrating InSb nanowires with other materials could potentially unfold novel devices with distinctive functionality. A prominent example is the combination of InSb nanowires with superconductors for the emerging topological particles research. Here, the combination of the II–VI cadmium telluride (CdTe) with the III–V InSb in the form of core–shell (InSb–CdTe) nanowires is investigated and potential applications based on the electronic structure of the InSb–CdTe interface and the epitaxy of CdTe on the InSb nanowires are explored. The electronic structure of the InSb–CdTe interface using density functional theory is determined and a type-I band alignment is extracted with a small conduction band offset ( $\leq 0.3$  eV). These results indicate the potential application of these shells for surface passivation or as tunnel barriers in combination with superconductors. In terms of structural quality, it is demonstrated that the lattice-matched CdTe can be grown epitaxially on the InSb nanowires without interfacial strain or defects. These shells do not introduce disorder to the InSb nanowires as indicated by the comparable field-effect mobility measured for both uncapped and CdTe-capped nanowires.

- A. van der Weijden, M. van Hecke and W.L. Noorduin, Contraction and expansion of nanocomposites during ion exchange reactions, *Cryst.Growth Des.*, **22** (2022), No. 4, 2289-2293.

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The next generation of advanced functional materials can greatly benefit from methods for realizing the right chemical composition at the right place. Nanocomposites of amorphous silica and metal carbonate nanocrystals ( $\text{BaCO}_3/\text{SiO}_2$ ) form an attractive starting point as they can straightforwardly be assembled in different controllable three-dimensional (3D) shapes, while the chemical composition of the nanocrystals can be completely converted via ion exchange. Nevertheless, it is still unknown how nanoscopic changes in the lattice volume of the nanocrystals translate to changes in the microscopic dimensions of 3D  $\text{BaCO}_3/\text{SiO}_2$  structures during ion exchange. Here, we demonstrate that the microscopic shape adapts to contraction and expansion of the atomic spacing of nanocrystals. Starting from  $\text{BaCO}_3/\text{SiO}_2$ , we systematically decrease and increase lattice volumes by converting the  $\text{BaCO}_3$  nanocrystals into a range of chalcogenides and perovskites. Based on geometrical analysis, we obtain a precise prediction for how the microscopic nanocomposite volume follows the change in nanoscopic crystal volume. The silica matrix facilitates mechanical flexibility to adapt to nanoscopic volume changes, while preserving the 3D morphology and fine details of the original composite with high fidelity. The versatility and predictability of shape-preserving conversion reactions open up exciting opportunities for using nanocomposites as functional components.

- C.T. van Campenhout, D.N. ten Napel, M. van Hecke and W.L. Noorduin, Rapid formation of uniformly layered materials by coupling reaction–diffusion processes with mechanical responsiveness, *PNAS*, **119** (2022), No. 39, e2123156119: 1-6.

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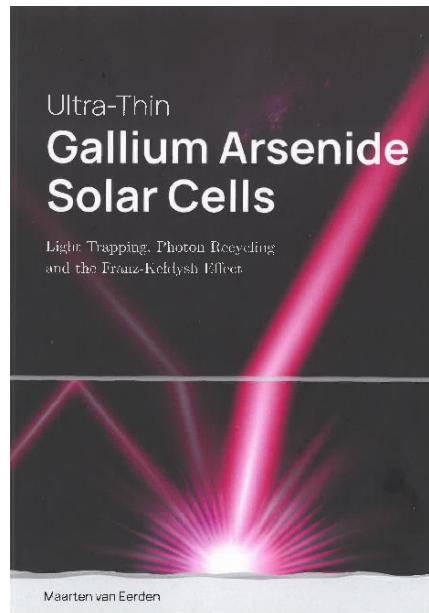
Equidistant layering of materials is central to the outstanding performance of biological minerals, such as nacre and bone, and offers exciting opportunities for classes of artificial materials with advanced functionalities. We demonstrate the self-organization of highly regular band patterns by embedding reaction–diffusion processes in mechanically responsive hydrogels. The mechanical deformation of the gel automatically regulates the local reactions conditions such that the reaction–diffusion process spontaneously generates equidistantly spaced layers. The simplicity, tunability, and generality of our self-organization strategy open exciting opportunities for exploiting reaction–diffusion processes toward fabricating components with advanced optical, mechanical, and thermal functionalities. Moreover, the here-introduced mechano-regulated chemical transport mechanism can impact our ability to understand and control pattern formation in complex and living matter.

## PhD theses

- Maarten van Eerden, Ultra-thin Gallium Arsenide solar cells –Light trapping, Photon recycling and the Franz-Keldysh effect.  
 PhD defense: 16 May 2022, Radboud Universiteit, Nijmegen

Promotor: Prof. dr. Elias Vlieg

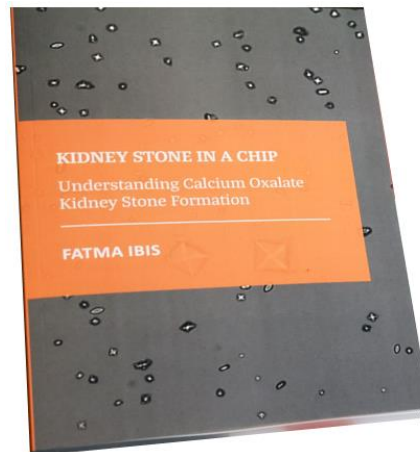
Co-promotor: Dr. ir. J.J. Schermer



Solar cells can be produced from a wide variety of different materials. The highest efficiencies are achieved in solar cells based on III-V semiconductors, such as gallium arsenide (GaAs). Therefore, these cells exhibit high power-to-weight ratios, making them especially suited for unmanned aerial vehicles and space applications. However, the production costs for these cells are high, due to the expensive crystalline substrates required as production template and the slow, batch-process epitaxial growth using high-cost precursor materials. One strategy to reduce the fabrication costs and simultaneously increase the tolerance of these solar cells for the harsh conditions in space is to make the absorber layer significantly thinner, creating so-called ‘ultra-thin’ solar cells. This reduces the material costs, increases the growth throughput and improves the radiation hardness by making the cell performance less susceptible to radiation-induced degradation. However, ultra-thin solar cells absorb less sunlight and therefore typically have a lower efficiency. These cell designs therefore require optical structures that increase the path length of photons by ‘trapping’ them inside the absorber layer. Such a light-trapping scheme uses textured interfaces, for example at the rear mirror, to scatter incident photons into wide angles and exploit total internal reflection to trap light inside the material and thereby increase the absorptivity of the solar cell. For ultra-thin GaAs solar cells, these light-trapping schemes often have several drawbacks, such as increased fabrication complexity or additional parasitic losses that degrade the device performance. This thesis describes the development, fabrication and simulation of ultra-thin GaAs solar cells, demonstrating a novel and simple approach to implement light trapping in these cells. Based on this approach, 300-nm-thick GaAs solar cells with a record efficiency of 21.4% are fabricated. For the first time in a solar cell, the Franz-Keldysh effect is demonstrated to have a significant impact on the performance metrics of these devices. Lastly, by developing a comprehensive framework that consistently models both absorption and emission, photon recycling and its impact on device performance is studied in detail, with an emphasis on ultra-thin GaAs solar cells.

- Fatma Ibis, [Kidney Stone in a Chip. Understanding calcium oxalate kidney stone formation.](#)  
 PhD defense: 8 June 2022, Delft University of Technology

Promotor: Prof. dr. ir. J.T. Padding  
 Co-promotor: Dr. H.B. Eral



Kidney stone formation is a global health problem with increasing prevalence. Stone formation is a physicochemical process involving crystallization of inorganic salts in the presence of biological constituents in the urinary system. To inhibit kidney stone formation, a better understanding of the underlying physicochemical mechanism of stone formation in the kidney is required.

In this thesis, the solubility, nucleation and growth of calcium oxalate (CaOx), the most common inorganic constituent of kidney stones, were studied under different conditions such as ion concentration, pH value, and also the role of inhibitors in water or artificial urine was investigated. The first step towards this work was obtaining the solubility curve of calcium oxalate monohydrate (COM) in the solvent, such as ultrapure water and different buffers, to elucidate the physicochemical conditions which can cause the kidney stone formation (Chapter 2).

Beside the solubility study, advanced technology to observe crystal formation in small scale and a very short time was needed. The volume, structure and flow properties inside the kidney inspired us to use microfluidic technology with comparable volume and flow rate. The developed microfluidic devices that mimic pathways in the human kidney were used to study the nucleation and growth of calcium oxalate crystals. The developed devices rendered an alternate perspective to the study of kidney stone formation and showed that microfluidics can provide precise, simple and fast detection of stone formation under various experimental conditions.

Initially, the designed microfluidic device allowed us to build a testing platform for the study of nucleation kinetics of CaOx inside isolated environments provided by droplets. Preliminary experiments were performed by dissolving calcium chloride and sodium oxalate in ultrapure water. The aqueous solution, containing the ions, forms the droplet phase and oil were used as the continuous phase. Altering the pH values, as well as increasing the concentration of additives such as magnesium and osteopontin (OPN), were shown to slow down the nucleation kinetics, or even inhibit nucleation (Chapter 3).

Next, the nucleation kinetics of CaOx was studied in artificial urine with varying concentrations of oxalate and, hyaluronic acid (HA), a protein commonly found in urine. The results showed that higher oxalate concentrations favored the formation of calcium oxalate dihydrate (COD), the metastable form, over COM, the most stable form. Additionally, COD was the fastest nucleating form in droplets under the conditions studied. An increasing concentration of HA at fixed calcium and oxalate concentrations favored the nucleation of COM. If COM nucleated first in the droplet, COD was not formed within the experimental time scale. However, in droplets where COD appeared first, COM crystals were observed later (Chapter 4).

Finally, the growth of CaOx in a microfluidic device, mimicking the geometry of a kidney collecting duct under flow conditions relevant for kidney stone formation, was studied. Calcium and oxalate ions were brought in contact in ultrapure water and artificial urine. The growth of CaOx crystals was measured as a function of fluid flow rate, the molar ratio of calcium and oxalate and the addition of OPN. COM was mainly seen in ultrapure water, while COD was found in artificial urine. OPN was shown to slow down the kinetics of both COM and COD crystals in ultrapure water and artificial urine, furthermore, the highest OPN concentration inhibit both crystal types in both solutions. Flow velocity did not affect the growth of COM and COD in ultrapure water and artificial urine within the range studied (Chapter 5).

