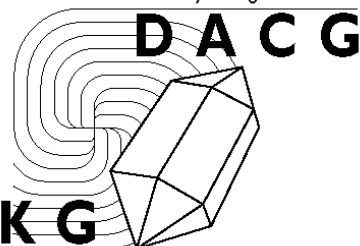


FACET

dutch association for crystal growth



NVKG

nederlandse vereniging voor kristalgroei

DACG NEWSLETTER

September 2020

issue 2

FACET

Newsletter of the Dutch

Association for Crystal Growth

(DACG), section of the KNCV and

the NNV.

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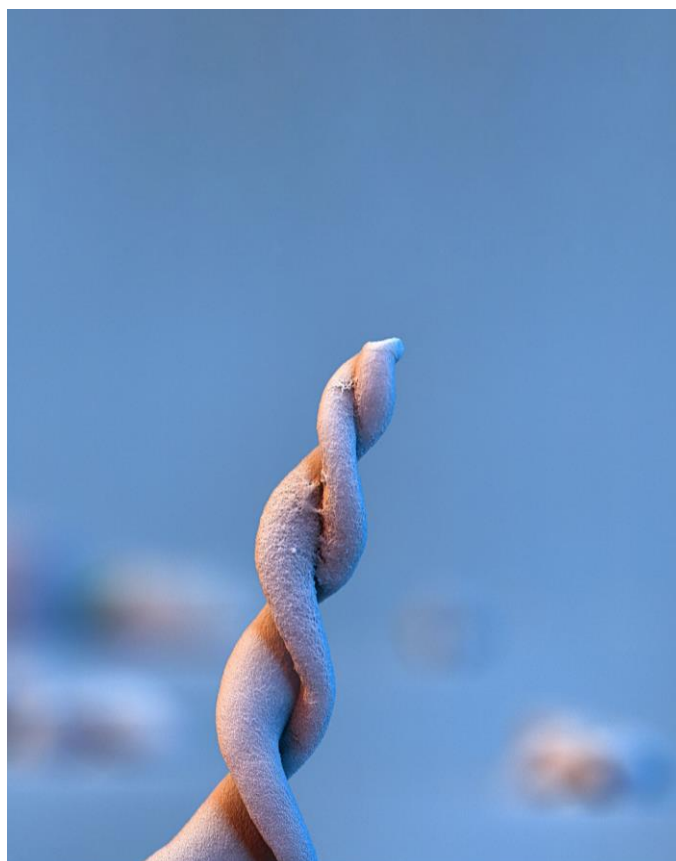
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DACG board

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

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

Cover figure

Here, Lukas Helmbrecht and co-workers present self-assembled, microscopic $\text{BaCO}_3/\text{SiO}_2$ double helices, which integrate directional emission and enantiomorph-specific circular retardance. This optical response emerges from the arrangement of nanoscopic mineral crystallites in the microscopic helix, and demonstrates how bottom-up assembly can achieve ordering across multiple length scales to form complex functional materials. [Imaged by Stefan Diller – Scientific Photography – Wuerzburg]

From the editor

Dear all,

I hope that you all are faring well. As you will see in this newsletter, the virus also has impact on the DACG activities. Read the details in “From the DACG Chairman” on page 5.

Do not forget to sign in for the annual meeting, which will be held online on Friday October 9th 12:00-13:30.

Regarding our 50th anniversary in 2022, we would like to ask you to have a look in your archives and send me photos that highlight 50 years of crystal growth events in the Netherlands, including pictures of your historical crystal growth or crys-tallization installations.

As always, it is easy to contribute to the FACET: recently published articles and theses, photos for cover figure, relevant announcements, ... Contributions may be delivered by mail, [e-mail](#), or telephone. Your ideas are welcome, please notify the editor: [Marketta Uusi-Penttilä](#)

Keep safe!

Marketta Uusi-Penttilä

Upcoming events

- Digitaal KNCV-event “[Avond van de Chemie](#)”, 8 October 2020, Eindhoven
 - [DACG Annual Meeting](#), 9 Oct 2020 12:00-13:30 , Online
 - [DACG Spring Meeting](#), Apr 2021, tbd.
-

From the DACG Chairman

Dear DACG-members,

Due to the current COVID-19 situation, the DACG Board has regretfully decided to cancel the planned DACG symposium in Geleen.

The local meeting room can only host 15 people, given the social distancing regulations. This small number limits the possibilities for the participants to meet each other in an open and friendly atmosphere, as we know from previous meetings.

Furthermore, a lab visit, which is a standard item on the annual meeting, is also not possible.

We would like to thank Pieter Vonk and his DSM-colleagues offering us the opportunity to organize a symposium on their premises.

The next possibility would be to organize an on-line event. However, we decided that this was not a desired option, since in our opinion the effort of the speakers to prepare their lecture and the attention and interaction that they will receive during an online presentation are not well balanced.

The DACG board will organize an on-line annual meeting according to the regular agenda. In this meeting, we will discuss the DACG annual report, the financials and we will announce the new cycle for the KNCV Piet Benema Crystal Growth Award 2021.

More information about the agenda and how to participate see page 6.

Although we could not organize a DACG-meeting in 2020, the board is motivated to plan new meetings in 2021.

We hope to meet all of you at the on-line annual meeting, or at the Spring meeting 2021.

On behalf of the DACG

Hans te Nijenhuis
Chairman

Membership

Becoming a member of the DACG is easy: send an e-mail message to [Antoine van der Heijden](#).

The annual membership fee in 2020 is € 15 for professionals, € 10 for 65+ and € 5 for (PhD) students.

Participating in one of the biannual symposia for the first time automatically includes a membership for the ongoing and following year. Members also participate our symposia for a reduced rate.

Announcement KNCV Piet Bennema Prize for Crystal Growth

Every three years the Dutch Association for Crystal Growth DACG distinguishes a young researcher with the KNCV Piet Bennema Award for Crystal Growth for his 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 similar importance 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

For the award of the prize both young Dutch and non-Dutch are eligible 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 dissertation must have been successfully defended at a Dutch university in the three years prior to the closing of the submission deadline (**1 May 2018 – 30 April 2021**). 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 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 KNCV Piet Bennema Prize for Crystal Growth is from **1 October 2020 to 30 April 2021**.

Award presentation

The KNCV Piet Bennema Award for Crystal Growth is awarded by the KNCV Board on the recommendation of the DACG Board. To this end, the board of the DACG appoints an assessment committee of three experts, who will test the candidates 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 2021.

On behalf of the board of the DACG

Prof. dr. A.E.D.M. van der Heijden

Secretary DACG

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Regulations for the KNCV Piet Bennema Prize for Crystal Growth

1. The Board of the KNCV awards a prize once every three years, consisting of a certificate and a sum of € 1000 to a young researcher for high-level scientific research in the field of crystal growth.
2. 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 similar importance to a thesis. The dissertation must be successfully defended at a Dutch university during the three-year period preceding the selection procedure. The scientific publications should also have appeared in the previous three-year period.
3. The prize will be awarded by the KNCV Board on the basis of a recommendation issued by the Board of the Netherlands Association for Crystal Growth. If the board of the association does not nominate a candidate, no prize will be awarded.
4. The KNCV Board may adopt or reject the recommendation referred to under 3. above. In the latter case the prize is not awarded.
5. Researchers who have carried out their research largely at a Dutch university or at a Dutch company are eligible for the award of the certificate.
6. The requirements for the award are that the candidate must have shown great competence as a researcher as well as scientific originality and productivity. In addition, he / she must have a good understanding of the problems of the field.
7. The Board of the Dutch Association for Crystal Growth ensures that all activities in the context of points 1 to 6 of these regulations are carried out.
8. The Board of the Dutch Association for Crystal Growth will be supported in its work by three experts, from whom it can be expected that they have a good overview of the work of researchers in the field of crystal growth. The experts provide their advice in writing, with documentation, such as publications. Members of the assessment committee cannot nominate candidates themselves.
9. The presentation of the KNCV Piet Bennema Prize for Crystal Growth takes place during the annual meeting of the Dutch Association for Crystal Growth. Justification of the award will be published after the award ceremony in the C2W.

DACG Annual Meeting

9 October 2020 12:00-13:30, online via MS Teams

1. Opening
2. Finalize agenda
3. Minutes Annual meeting 4 October 2019, Eindhoven
4. Documents sent / received: Report financial audit committee 2019
5. Annual Report Oct 2019 – Oct 2020
6. Financial
 - (a) Annual Report Oct 2019 – Oct 2020
 - (b) Report Financial Audit Committee
 - (c) Budget proposal 2020-2021
7. Board

Role	2019 – 2020	Appointment deadline
President	Hans te Nijenhuis	Step down Oct 2021
Secretariat	Antoine van der Heijden	Step down Oct 2022
Treasurer	Pieter Vonk	Step down Oct 2021
Webmaster	Hugo Meekes	Step down Oct 2020 (re-electable)
FACET	Marketta Uusi-Penttilä	Step down Oct 2020 (re-electable)

Two of the DACG board members step down, but are 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), ultimately by 30 September 2020.

8. 2021: KNCV Piet Bennema Crystal Growth Award
9. 2022: DACG 50 years
10. Status Stichting
11. Activities 2020 – 2021
 - a. Digital KNCV-event “Avond van de Chemie”, 8 October 2020, Eindhoven
 - b. NNV-adviesraadvergadering, 9 December 2020, Utrecht (section boards will be invited)
 - c. April 2021: DACG spring meeting, University of Utrecht, date to be decided
 - d. October 2021: Annual meeting + symposium, date/location to be announced
12. Questions before closure of meeting
13. Adjourn

To receive the MS Teams meeting invitation, please register by sending an email titled “Registration for DACG Annual Meeting 2020” to a.e.d.m.vanderheijden@tudelft.nl **by 2 October 2020.**

Annual Report Dutch Association for Crystal Growth (DACG) October 2019 – October 2020

Secretariat

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Members

The total number of members is 48 (this includes 8 “lifetime” members and 14 “calendar year” members that have been offered membership in 2020 through the registration fee for the Fall Meeting in October 2019¹). In addition to this number, there are a few tens of members from whom payment of contribution is still pending/expected.

Board

The DACG Board is summarized in the table below. The Board had six meetings: one face-to-face meeting (hosted by Radboud University Nijmegen) and five telcon/video meetings.

Role	2019 – 2020	Appointment deadline	E-mail
President	Hans te Nijenhuis	Step down Oct 2021	hans.te.nijenhuis@panalytical.com
Secretary	Antoine van der Heijden	Step down Oct 2022	a.e.d.m.vanderheijden@tudelft.nl
Treasurer	Pieter Vonk	Step down Oct 2021	pieter.vonk@dsm.com
Webmaster	Hugo Meekes	Step down Oct 2020 (re-electable)	h.meekes@science.ru.nl
FACET	Marketta Uusi-Penttilä	Step down Oct 2020 (re-electable)	muusipenttila@nl.aspenpharma.com

FACET Newsletter

The DACG Newsletter, FACET, was issued in March and September 2020. Dr 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.

¹ The Spring meeting in April 2020 had to be cancelled, so no additional “calendar year” members resulted from this event.

Website

The DACG website (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 Dr Hugo Meekes (h.meekes@science.ru.nl).

Meetings / excursions organized by DACG

On October 4, 2019 the Fall Symposium and annual meeting were held in Eindhoven, hosted by ThermoFisher Scientific and organized by Nico Clemens.

On April 3, 2020 the DACG intended to hold its Spring Meeting, hosted by University of Utrecht Enschede and co-organized by prof Alfons van Blaaderen. Unfortunately, this symposium had to be cancelled due to the Covid-19 outbreak.

Activities relevant to DACG community

A shortlist of past activities relevant to the DACG community:

- 3 October 2019: KNCV-event "Avond van de Chemie", Zwolle, Theater Odeon; more information see: <https://www.kncv.nl/bijeenkomsten/542/avond-van-de-chemie-2019/about#.XVbFjnduLmJ>
- 10 December 2019: NNV Adviesraadvergadering, Utrecht (Hans te Nijenhuis and Antoine van der Heijden attended this meeting on behalf of DACG)
- 3 April 2020: DACG Spring Meeting; cancelled due to Covid-19
- 9 October 2020: DACG Fall Meeting (on-line)

DACG's 50th 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 will celebrate its 50th anniversary. A commission, led by Prof Elias Vlieg, has been founded in 2019 that will start the preparations for organizing an international symposium similar to the BRIDGE symposia held in the past. A date for this event is 23-25 March 2022 in the Aula of the University of Amsterdam (Oude Lutherse Kerk, Singel 411, Amsterdam). Next to NL, UK and Germany, we also intend to invite our Belgian, French and Irish colleagues. Furthermore, the DACG board is looking for other possibilities to celebrate half a century of crystal growth in the Netherlands. DACG members who would like to share their ideas or support the DACG board with the organization of the 50th anniversary of the DACG are most welcome. Please contact the secretary.

Upcoming activities

- 8 October 2020: digitale "Avond van de Chemie" (KNCV event); more information: <https://www.kncv.nl/bijeenkomsten/704/avond-van-de-chemie-2020/about#.XpnPx3duLVI>
- 9 December 2020: NNV Adviesraadvergadering, Utrecht (section boards will be invited)
- April 2021: DACG Spring Meeting; University of Utrecht; date to be decided
- October 2021: DACG Fall Meeting; date/location to be decided

Recent publications

- L. Helmbrecht, M. Tan, R., Röhrich, M.H. Bistervels, B.O. Kessels, A.F. Koenderink, B. Kahr, W.L. Noorduin, [Directed Emission from Self-Assembled Microhelices](#). *Adv. Funct. Mater.* 2020, **30**, 1908218.

Affiliations

- AMOLF, Science Park 104, Amsterdam, 1098XG The Netherlands
- Department of Chemistry, New York University, 100 Washington Square East, New York City, NY, 10003-6688 USA
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Bottom-up assembly can organize simple building blocks into complex architectures for light manipulation. The optical properties of self-assembled polycrystalline barium carbonate/silica double helices are studied using fluorescent Fourier and Mueller matrix microscopy. Helices doped with fluorescein direct light emission along the long axis of the structure. Furthermore, light transmission measured normal and parallel to the long axis exhibits twist sense-specific circular retardance and waveguiding, respectively, although the measurements suffer from depolarization. The helices thus integrate highly directional emission with enantiomorph-specific polarization. This optical response emerges from the arrangement of nanoscopic mineral crystallites in the microscopic helix, and demonstrates how bottom-up assembly can achieve ordering across multiple length scales to form complex functional materials.

- A.R. Mol, R.D. van der Weijden, J.B.M. Klok, C.J.N. Buisman, [Properties of Sulfur Particles Formed in Biodesulfurization of Biogas](#), *Minerals* 2020, **10**(5), 433.

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In the biodesulfurization (BD) process under halo-alkaline conditions, toxic hydrogen sulfide is oxidized to elemental sulfur by a mixed culture of sulfide oxidizing bacteria to clean biogas. The resulting sulfur is recovered by gravitational settling and can be used as raw material in various industries. However, if the sulfur particles do not settle, it will lead to operational difficulties. In this study, we investigated the properties of sulfur formed in five industrial BD facilities. Sulfur particles from all samples showed large differences in terms of shape, size, and settleability. Both single crystals (often bipyramidal) and aggregates thereof were observed with light and scanning electron microscopy. The small, non-settled particles account for at least 13.6% of the total number of particles and consists of small individual particles with a median of 0.3 μm . This is undesirable, because those particles cannot be removed from the BD facility by gravitational settling and lead to operational interruption. The particles with good settling properties are aggregates (5–20 μm) or large single crystals (20 μm). We provide hypotheses as to how the differences in sulfur particle properties might have occurred. These findings provide a basis for understanding the relation between sulfur particle properties and formation mechanisms.

- M.M.J. van Rijt, B.M. Oosterlaken, R.R.M. Joosten, L.E.A. Wijkhuijs, P.H.H. Bomans, H. Friedrich, G. de With, [Counter-ion influence on the mechanism of HMTA-mediated ZnO formation](#), *CrystEngComm* 2020, Advance Article.

Affiliation

- Laboratory of Physical Chemistry, Center for Multiscale Electron Microscopy, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P. O. Box 513, 5600 MB Eindhoven, The Netherlands

Crystalline materials are often formed via transient phases. Here we focus on ZnO as a widely used and investigated material for technological applications. Although the literature for the wet chemical synthesis of ZnO is extensive, its formation pathway using these strategies has gained limited attention so far and is poorly understood. To gain insight in these pathways, a HMTA-mediated ZnO synthesis protocol with a variety of zinc salts was employed using in-situ pH measurements combined with discrete cryoTEM and SEM sampling studies, in addition to more typical pXRD and SEM product analysis. These results indicate a significant counter-ion effect on the reaction product. Using acetate, nitrate, chloride and sulphate as counter-ions all result first in the formation of a layered zinc hydroxy salt (LZHS), the exact composition of which depends on the counter-ion. Rather stable LZHSs are formed using chloride and sulphate, preventing the eventual formation of ZnO. Only acetate and nitrate result in the formation of ZnO. For acetate, ZnO is preferably grown in-dispersion, while for nitrate it is formed on exposed solid interfaces to the reaction medium (on-surfaces). For the latter the nucleation of its LZHS precursor requires an additional incubation time, resulting in heterogenous nucleation instead.

- S. Hanselman, I.T. McCrum, M.J. Rost, M.T.M. Koper, [Thermodynamics of the formation of surface PtO₂ stripes on Pt\(111\) in the absence of subsurface oxygen](#), *Phys. Chem. Chem. Phys.* 2020, **22**(19), 10634-10640.

Affiliation

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- Huygens-Kamerlingh Onnes Laboratory, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands

This paper examines the thermodynamics of PtO₂ stripes formed as intermediates of Pt(111) surface oxidation as a function of the degree of dilation parallel to the stripes, using density functional theory and atomistic thermodynamics. Internal energy calculations predict 7/8 and 8/9 stripe structures to dominate at standard temperature and pressure, which contain 7 or 8 elevated PtO₂ units per 8 or 9 supporting surface Pt atoms, respectively. Moreover, we found a thermodynamic optimum with respect to mean in-stripe Pt–Pt spacing close to that of α -PtO₂. Vibrational zero point energies, including bulk layer contributions, make a small but significant contribution to the stripe free energies, leading to the 6/7 stripe being most stable, although the 7/8 structure is still close in free energy. These findings correspond closely to experimental observations, providing insight into the driving force for oxide stripe formation and structure as the initial intermediate of platinum surface oxidation, and aiding our understanding of platinum catalysts and surface roughening under oxidative conditions.

- X. Zhu, G.H. ten Brink, S. de Graaf, B.J. Kooi, G. Palasantzas, [Gas-Phase Synthesis of Tunable-Size Germanium Nanocrystals by Inert Gas Condensation](#), *Chem. Mater.* 2020, **32**(4), 1627–1635.

Affiliation

- Zernike institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Size-dependent optical properties of germanium (Ge) nanocrystals (NCs) make them a desirable material for optoelectronic applications. So far, the synthesis of ligand-free and tunable-size Ge NCs by inert gas condensation has been scarcely reported. In this work, we introduce a gas-phase approach to synthesize quantum-confined Ge NCs by inert gas condensation, where the size of the Ge NCs can be readily tuned by controlling the thickness of a Cu plate supporting the Ge target. As explained by simulations using the finite element method, the magnetic field configuration above the target can be manipulated by varying the thickness of the Cu backing plate. In-depth analysis based on transmission electron microscopy (TEM) results reveals the morphology and crystalline structure of Ge NCs. X-ray photoelectron spectroscopy has proven the formation of a substoichiometric Ge oxide shell for the as-deposited Ge NCs. In addition, Raman spectroscopy indicated peak shifts according to the phonon confinement model that yielded nanoparticle sizes in a good agreement with the TEM results. Furthermore, the quantum confinement effect for Ge NCs was demonstrated by analysis of the absorption (UV–vis–NIR) spectrum, which indicated that the band gap of the Ge NCs was increased from ~ 0.8 to 1.1 eV with decreasing size of Ge NCs. Comparison with theory shows that the quantum confinement effect on the band gap energy for different-sized Ge NCs follows the tight-binding model rather well.

- Maarten van Eerden, Jasper van Gastel, Gerard J. Bauhuis, Peter Mulder, Elias Vlieg and John J. Schermer, [Observation and implications of the Franz-Keldysh effect in ultrathin GaAs solar cells](#), *Progress in Photovoltaics*, **28** (2020) 779-787.

Affiliations

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The Franz-Keldysh effect is shown to have a significant impact on the external quantum efficiency (EQE) spectra of ultrathin GaAs solar cells, leading to voltage-dependent above-bandgap oscillations and subbandgap tails. The implications of this observation for the use of the photovoltaic reciprocity relation are discussed. It is demonstrated that the radiative VOC limit of ultrathin solar cells employing light management schemes can be underestimated by more than 25 mV, leading to an overestimation of the external luminescent efficiency by a factor of 3.

- W. de Poel, S.J.T. Brugman, K.H.A. van de Ven, A. Gasseling, J. de Lange, E.R. Townsend, A.H.J. Engwerda, M. Jankowski, M. Blijlevens, B.L. Werkhoven, J. Drnec, F. Carla, R. Felici, A. Tuladhar, N.M. Adhikari, J.J. De Yoreo, J.A.A.W. Elemans, W.J.P. van Enkevort, A.E. Rowan and E. Vlieg, [Organothiol monolayer formation directly on muscovite mica](#), *Angew. Chem. Int. Ed.*, **59** (2020) 2323-2327.

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- Physical Sciences Division, Pacific Northwest National Laboratory, Richland, WA99352 (USA)

Organothiol monolayers on metal substrates (Au, Ag, Cu) and their use in a wide variety of applications have been extensively studied. Here, the growth of layers of organothiols directly onto muscovite mica is demonstrated using a simple procedure. Atomic force microscopy, surface X-ray diffraction, and vibrational sum-frequency generation IR spectroscopy studies revealed that organothiols with various functional endgroups could be self-assembled into (water) stable and adaptable ultra-flat organothiol monolayers over homogenous areas as large as 1 cm². The strength of the mica–organothiol interactions could be tuned by exchanging the potassium surface ions for copper ions. Several of these organothiol monolayers were subsequently used as a template for calcite growth.

- M.M.H. Smets, E. Kalkman, A. Krieger, P. Tinnemans, H. Meekes, E. Vlieg, H.M. Cuppen, [On the mechanism of solid-state phase transitions in molecular crystals - The role of cooperative motion in \(quasi\)racemic linear amino acids](#), *IUCrJ* **7** (2020) 331-34.

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During single-crystal-to-single-crystal (SCSC) phase transitions, a polymorph of a compound can transform to a more stable form while remaining in the solid state. By understanding the mechanism of these transitions, strategies can be developed to control this phenomenon. This is particularly important in the pharmaceutical industry, but also relevant for other industries such as the food and agrochemical industries. Although extensive literature exists on SCSC phase transitions in inorganic crystals, it is unclear whether their classifications and mechanisms translate to molecular crystals, with weaker interactions and more steric hindrance. A comparative study of SCSC phase transitions in aliphatic linear-chain amino acid crystals, both racemates and quasi-racemates, is presented. A total of 34 transitions are considered and most are classified according to their structural change during the transition. Transitions without torsional changes show very different characteristics, such as transition temperature, enthalpy and free energy, compared with transitions that involve torsional changes. These differences can be rationalized using classical nucleation theory and in terms of a difference in mechanism; torsional changes occur in a molecule-by-molecule fashion, whereas transitions without torsional changes involve cooperative motion with multiple molecules at the same time.

- A.E.F. de Jong, V. Vonk, M. Bockowski, I. Grzegory, V. Honkimäki and E. Vlieg, [Complex geometric structure of a simple solid-liquid interface: GaN\(0001\)-Ga](#), *Phys. Rev. Lett.* **124** (2020) 086101, 1-5.

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The equilibrium atomic interface structure between Ga and GaN(0001) is shown to contain substrate surface vacancies followed by substrate-induced layering and preferential lateral ordering in the liquid. The uncovered presence of point defects, in the form of vacancies at both sides of the solid-liquid interface, is an important structural feature which governs the local physical properties. Our x-ray diffraction study reveals that the layering is very stable and persists up to a temperature of 1123 K and a nitrogen pressure of 32 bar. The Ga layer spacing agrees remarkably well with the Friedel oscillation period for this system.

- S.J.T. Brugman, A.B. Ottenbros, F. Megens, W.J.P. van Enckevort and E. Vlieg, [Epitaxy of rhodochrosite \(MnCO₃\) on muscovite mica and its relation with calcite \(CaCO₃\)](#), *Cryst. Growth Des.* **20** (2020) 4802-4810.

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The flatness of muscovite mica makes it a convenient substrate to study epitaxy. We have analyzed the growth of rhodochrosite (MnCO₃) crystals in solution and on muscovite mica. Growth at high supersaturations occurs via the formation of amorphous MnCO₃, which over time transforms into the crystalline form. In the presence of muscovite mica, epitaxial rhodochrosite crystals with a size of approximately 1 μm form. These crystals are kinetically roughened, because of the high supersaturation. The lattice match between MnCO₃ and muscovite was found not to be the main reason for epitaxy. If the growth experiment is performed twice, the original epitaxial MnCO₃ crystals are overgrown by many small crystallites. Similarly, spherical MnCO₃ crystals with many overgrown facets can be formed on a muscovite surface that is exposed to humidity or by using a higher MnCO₃ supersaturation. A comparison with calcite shows that epitaxy strongly depends on initial supersaturation for both carbonates. In contrast to previous studies, we find that at the right supersaturation, epitaxial calcite crystal growth is possible on freshly cleaved muscovite.

- S.J.T. Brugman, P. Raiteri, P. Accordini, F. Megens, J.D. Gale and E. Vlieg, [Calcite \(104\) surface - electrolyte structure: a 3D comparison of surface X-ray diffraction and simulations](#), *J. Phys. Chem. C* **124** (2020) 18564-18575.

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Adsorption and incorporation of ions are known to influence the morphology and growth of calcite. Using surface X-ray diffraction, the interfacial structure of calcite in contact with CaCO_3 , MgCl_2 , CaCl_2 , and BaCl_2 solutions was determined. All of these conditions yield a comparable interfacial structure, meaning that there is no significant ion adsorption on the terraces under the investigated conditions. This allows, for the first time, a thorough comparison in all three dimensions with state-of-the-art computer simulations, involving molecular dynamics based on both density functional theory (DFT) and two different force field models. Additionally, the simulated structures are used to calculate the corresponding structure factors, which in turn are compared to those obtained from experiment, thereby avoiding the need for fitting or subjective interpretation. In general, there is a good agreement between experiment and the simulations, although there are some small discrepancies in the atomic positions, which lead to an inadequate fit of certain features characteristic of the structure of water at the interface. Of the three simulation methods examined, the DFT results were found to agree best with the experimental structure.

- J.J. Devogelaer, H. Meekes, P. Tinnemans, E. Vlieg, R. de Gelder, [Cocrystal prediction by artificial neural networks](#), *Angew. Chem. Int. Ed.* 10.1002/anie.202009467.

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A significant amount of attention has been given to the design and synthesis of cocrystals by both industry and academia because of its potential to change a molecule's physicochemical properties. Yet, difficulties arise when searching for adequate combinations of molecules (or cofomers) to form cocrystals, hampering the efficient exploration of the target's solid-state landscape. This paper reports on the application of a data-driven cocrystal prediction method, based on two types of artificial neural network models and cocrystal data present in the Cambridge Structural Database. The models accept pairs of cofomers and predict whether a cocrystal is likely to form. By combining the output of multiple models of both types, our approach shows to have excellent performance on the proposed cocrystal training and validation sets, and has an estimated accuracy of 80% for molecules for which previous cocrystallization data is unavailable.