CRYSTAL GROWTH & DESIGN

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Editorial

Women Researchers at the Forefront of Crystal Engineering

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This profile series highlights work in crystal engineering by authors who are cisgender or transgender women. The inspiration for this virtual issue on Women Researchers at the Forefront of Crystal Engineering evolved out of a discussion at a meeting of *Crystal Growth & Design* editors in late June 2022. Shortly before the meeting, Aurora J. Cruz-Cabeza, Professor of Chemistry at Durham University and former Topic Editor of *CG&D*, raised the issue of gender bias in chemistry publishing by bringing to our attention a 2020 bioRxiv preprint, which was published as a Perspective in *ACS Chemical Biology*.[1] The Perspective demonstrates the underrepresentation of women in chemistry publishing, and it sparked honest conversations about the experiences and bias that women may encounter throughout the research and publication process.

The *CG&D* editors already wanted to spotlight the valuable to contributions that women alongside other minority groups make to the field, and the initial path forward was outlined at this editors' meeting. We decided not to pursue a Virtual Special Issue of new content, to avoid placing an additional burden on women to write and submit a manuscript within a specified time window to be included. Rather, we decided to feature articles, communications, and reviews that women had already published in the pages of *CG&D*.

To maximize participation and to allow authors to self-identify and opt-in, all corresponding authors of *CG&D* articles published in the journal's January to December 2022 issues were contacted.[2] Corresponding authors and first authors who identify as women we invited to submit a link to their published article and, optionally, a photo of themselves and a brief statement about their experience as a researcher in crystal engineering. Through these statements, women could share their perspective on topics such as succeeding in academia, lessons learned through their journey, the importance of community support, and more. The statements have become an incredibly valuable part of the virtual issue and we thank these individuals for taking to share their stories, which we believe will inspire other women and other minority groups not only in the field of crystal engineering and design, but in the wider chemical sciences. These statements are available to read below.

The responses to this invitation are very encouraging. Thirty-eight first authors or corresponding authors submitted information for inclusion in the virtual issue, and these authors embody diversity in several dimensions. Academia, industry, and US national labs are represented, as are career stages from staff researcher to graduate student to full professor. The authors hail from 15 different countries, including some international collaboration.

We hope that you will be inspired by and join us in celebrating the contributions that women have made and will continue to make to the field. They are at the forefront of research in crystal engineering and will certainly drive further progress in years to come.

FAST $(Ce,Gd)_3Ga_2Al_3O_{12}$ SCINTILLATORS GROWN BY THE OPTICAL FLOATING ZONE METHOD

Tong Wu, Ling Wang, Yun Shi*, Tianzhao Xu, Hui Wang, Jinghong Fang, Jinqi Ni, Huan He, Chaoyue Wang, Bo Wan, Dongzhou Ding, Zhenzhen Zhou, Qian Liu, Qin Li, Jianding Yu, Xintang Huang*, Oleg. Shichalin, and E. K. Papynov

Cryst. Growth Des. **2022**, *22*(1), 180−190 (Article)

DOI: 10.1021/acs.cgd.1c00779

Dr. Yun Shi. Photo courtesy of Yun Shi.

In the past 3 years, I focused on the growth of scintillator crystals by the optical floating zone method. The method is one of the container-less technologies, which avoids impurities from crucibles and can grow crystals with very high melting points. It is faster than that of other crystal growth methods, which improves the efficiency of the development of new materials.

Yun Shi

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http://sourcedb.sic.cas.cn/zw/rck/201104/t20110425_3121065.html

Published: June 7, 2023

CONTROLLING THE π-STACK GROWTH DIRECTION IN ORGANIC π-CONJUGATED MICROCRYSTALS

Dorothy K. Jones and Nagarjuna Gavvalapalli*

Cryst. Growth Des. **2022**, *22*(1), 1−19 (Perspective)

DOI: 10.1021/acs.cgd.1c00993

When I started graduate school, I had no experience in crystal engineering or crystallography. As my thesis project evolved to include studying micro- and nanocrystals, I found myself having to learn a whole new branch of chemistry. I was incredibly lucky to have the support of the Georgetown University Chemistry Department community throughout that process. The crystallography staff, students, and faculty were all invaluable during my graduate experience, mentoring me and training me on new techniques.

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OCTAHEDRAL MOLYBDENUM CLUSTER-BASED SINGLE CRYSTALS AS FABRY−PÉROT MICRORESONATORS

Elena Segura-Sanchis, Roberto Fenollosa*, Isabelle Rodriguez, Yann Molard, Stéphane Cordier, Marta Feliz*, and Pedro Atienzar*

Cryst. Growth Des. **2022**, *22*(1), 60−65 (Communication)

DOI: 10.1021/acs.cgd.1c01144

Dr. Marta Feliz. Photo courtesy of Marta Feliz.

My experience in crystal engineering began during my PhD with the isolation of trinuclear group VI clusters. In this period, I immersed myself into crystallography, learned to be resilient in crystallization and was fascinated with the isolation of crystals and their morphologies. Nowadays, I continue working on the building block of transition metal materials and being captivated by the structures obtained, the interactions between atoms, and the assembly of the metal entities in the dimensional space through supramolecular interactions. In my experience, the combined X-ray and computational analysis of the geometrical and electronic features of the structures embedded in the crystal lattice gives me clues for potential catalytic sites. The isolation of single-crystal frameworks provides to me new inputs for adsorption and reactivity studies in heterogeneous conditions, and facilitates the determination of new optical properties, such as those derived from photoluminescence.

Marta Feliz
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CHIRAL 1D METAL−ORGANIC MATERIALS BASED ON Cu(II) AND AMINO ACID SCHIFF BASES

Carlos Cruz, Carla Gonzalez, Francisco Rubio, Juan Erices, Kerry Wrighton-Araneda, Diego Cortés-Arriagada, Diego Venegas-Yazigi, Nathalie Audebrand, and Verónica Paredes-García*

Cryst. Growth Des. **2022**, *22*(1) 237−250 (Article)

DOI: 10.1021/acs.cgd.1c00877

Prof. Verónica Paredes-García. Photo courtesy of Verónica Paredes.

Coordination polymers (CPs) based on transition cations (nd), as well as lanthanoids cations (4f), are a class of materials that offer an excellent platform to carry out highly applied research, also offering high adaptability to study different phenomena, depending on the chosen building blocks. The purpose is to develop new materials based mainly on strategic Chilean metals cations, which allow the generation of different materials characterized by presenting unique catalytic, electrical, or magnetic properties, also permitting the generation of multipurpose materials. The development of this area has allowed me to consolidate myself academically and as a researcher in the coordination polymers area. This is a product of perseverance, dedication, discipline at work, resilience to face challenges, and creativity to solve the usual obstacles of scientific and academic work, aptitudes and skills that have been developed throughout my career.

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MECHANOCHEMISTRY AS A TOOL FOR CRYSTALLIZING INACCESSIBLE SOLIDS FROM VISCOUS LIQUID COMPONENTS

Jesus Daniel Loya, Selena J. Li, Daniel K. Unruh, and Kristin M. Hutchins*

Cryst. Growth Des. **2022**, *22*(1), 285−292 (Article)

DOI: 10.1021/acs.cgd.1c00929

COCRYSTALLIZATION AND THERMAL BEHAVIORS OF THE MICROPOLLUTANTS GEMFIBROZIL, ACECLOFENAC, AND BISPHENOL A

Qixuan Zheng, Daniel K. Unruh, and Kristin M. Hutchins*
Cryst. Growth Des. **2022**, *22*(4), 2208−2217 (Article)
DOI: 10.1021/acs.cgd.1c01291

MOLECULAR MOTION AND LIGAND STACKING INFLUENCE THERMAL EXPANSION BEHAVIOR AND ARGENTOPHILIC FORCES IN SILVER COORDINATION COMPLEXES

Gary C. George III, Daniel K. Unruh, Ryan H. Groeneman, and Kristin M. Hutchins*
Cryst. Growth Des. **2022**, *22*(7), 4538−4545 (Article)
DOI: 10.1021/acs.cgd.2c00446

Dr. Kristen Hutchins. Photo courtesy of Kristen Hutchins.

I found the crystal engineering community to be supportive both as a student and faculty member. As a first-generation student and woman, succeeding in academia is not always easy. I am fortunate to have incredibly supportive mentors, both within the crystal engineering community and outside it. It is critical to identify good mentors for yourself who will help you learn how to succeed and be there when you need support. For example, most of us are familiar with frequent rejections (grants, papers). My mentors taught me early on that rejections happen and not to be too discouraged by them. Instead, use the opportunity to grow as a scientist or writer. I strive to provide the same supportive mentorship for my students. It is an exciting time to be in our field. Although crystal engineering has already been applied in impactful ways (e.g., drug development), I am confident we will continue to see the importance and impact of crystal engineering strategies applied to big world challenges.

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OPTIMIZATION OF AMORPHIZATION KINETICS DURING HOT MELT EXTRUSION BY PARTICLE ENGINEERING: AN EXPERIMENTAL AND COMPUTATIONAL STUDY

Dana E. Moseson, Ayse Eren, Kevin J. Altman, Isaac D. Corum, Mingyue Li, Yongchao Su, Zoltan K. Nagy, and Lynne S. Taylor*
Cryst. Growth Des. **2022**, *22*(1), 821−841 (Article)
DOI: 10.1021/acs.cgd.1c01306

Dr. Dana Moseson. Photo courtesy of Jeff Rattray.

Among the best advice ever given to me was to not say "no" immediately to new opportunities or ideas. While some opportunities may not align with your current path or future goals, sometimes they provide the best forums for personal growth, networking, and discovery of new science! This idea is well represented in a trilogy of articles I published in *Crystal Growth & Design*, which were inspired by and augmented by contributions of several amazing women in my network. Naila Mugheirbi and I imaged our first amorphous solid dispersion particles and discovered the most beautiful nanometer-scale crystalline domains that resulted from incomplete crystalline-to-amorphous phase transformation during processing (DOI: 10.1021/acs.cgd.8b01435). Based Lynne Taylor's insights into our initial transmission electron microscopy images, I developed controlled characterization methods and observed the role of intrinsic defects on the mechanistic pathways of crystal dissolution by diffusion and fragmentation (DOI: 10.1021/acs.cgd.9b00200). Ayse Eren and I then translated these concepts into experimental and computational studies of defect-based crystal dissolution kinetics during hot melt extrusion processing (DOI: 10.1021/acs.cgd.1c01306). Each of these remarkable women has shaped and developed me into a more well-rounded scientist and worked alongside me to push the boundaries of our scientific niche by ultimately connecting disparate fields of study into interesting new areas of particle engineering, crystallization, crystal dissolution, and pharmaceutical processing to prepare amorphous solid dispersions.

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DIGITAL DESIGN OF THE CRYSTALLIZATION OF AN ACTIVE PHARMACEUTICAL INGREDIENT USING A POPULATION BALANCE MODEL WITH A NOVEL SIZE DEPENDENT GROWTH RATE EXPRESSION. FROM DEVELOPMENT OF A DIGITAL TWIN TO IN SILICO OPTIMIZATION AND EXPERIMENTAL VALIDATION

Botond Szilágyi, Ayşe Eren, Justin L. Quon, Charles D. Papageorgiou, and Zoltán K. Nagy*
Cryst. Growth Des. **2022**, *22*(1), 497−512 (Article)
DOI: 10.1021/acs.cgd.1c01108

https://doi.org/10.1021/acs.cgd.3c00609
Cryst. Growth Des. 2023, 23, 3917−3930

Kutlu Ulgen, Ayşe Eren, and Elif Ozkirimli Olmez. Photo courtesy of Ayşe Eren.

I have always had a strong desire to learn and stay up to date with technological and scientific advancements, so I pursued an academic career. As the years rolled by I started understanding value of the support that I had from fellow scientists and advisers, specifically from ones I could relate to the most, women. I was lucky to have two great women professors (Elif Ozkirimli Olmez and Kutlu Ulgen) during my undergraduate and masters who supported me throughout my journey along with other researchers who supported me later in my career. These women created more opportunities and guidance probably more than they think they did, such as Lynne Taylor and Dana Moseson. I am thankful to them for giving me this opportunity. Now as I start mentoring younger researchers, I clearly see the need to increase the number of women in academia to not leave it to chance to feel connected, belong, and be felt.

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Ayşe Eren is also an author of the article featured in the previous profile.

ISOCYANIDE AND CYANIDE ENTITIES FORM ISOSTRUCTURAL HALOGEN BOND-BASED SUPRAMOLECULAR NETWORKS FEATURING FIVE-CENTER TETRAFURCATED HALOGEN···C/N BONDING

Alexander S. Mikherdov, Roman A. Popov, Andrey S. Smirnov, Anastasiya A. Eliseeva, Alexander S. Novikov, Vadim P. Boyarskiy, Rosa M. Gomila, Antonio Frontera, Vadim Yu. Kukushkin*, and Nadezhda A. Bokach*

Cryst. Growth Des. **2022**, *22*(10), 6079−6087 (Article)
DOI: 10.1021/acs.cgd.2c00686

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CENTRAL METALS TO GUIDE THE BANDGAP OF HOURGLASS-TYPE POLYOXOMETALATE HYBRIDS AS PHOTOCATALYST FOR THE REDUCTION OF Cr(VI)

Hao-Xue Bi, Lin Hou, Xiao-Yu Yin, Yuan-Yuan Ma*, and Zhan-Gang Han*

Cryst. Growth Des. **2022**, *22*(1), 738−746 (Article)
DOI: 10.1021/acs.cgd.1c01236

Prof. Yuan-Yuan Ma. Photo courtesy of Yuan-Yuan Ma.

Yuan-Yuan Ma received her BS degree in 2013 and PhD in Inorganic Chemistry from Northeast China Normal University in 2018. Currently, she is an Associate Professor in the College of Materials and Chemistry, Hebei Normal University. Her research interests are the design and synthesis of novel functional polyoxometalate-based crystalline materials and polyoxometalate-derived nanomaterials, and their applications in catalyst, photocatalysis, and electrocatalysis (e.g., HER, OER, CO_2RR).

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SELECTIVE LOADING OF XYLENE ISOMERS IN SELF-ASSEMBLED TRIPHENYLAMINE BIS-UREA MACROCYCLES

Dustin W. Goodlett, Ammon J. Sindt, Md Faizul Islam, Mark D. Smith, and Linda S. Shimizu*

Cryst. Growth Des. **2022**, 22 (2), 1017−1023 (Article)
DOI: 10.1021/acs.cgd.1c00846

Prof. Linda Shimizu. Photo courtesy of Linda Shimizu.

As someone who first moved into the area as an assistant professor, I have found the Crystal Engineering community to

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be welcoming and mentoring. Participating in crystal engineering-focused meetings such as GRC and ACA conferences highlighted the rigor and broad background of the participants. These are especially great meetings to bring my students as sharing results always results in lively discussions.

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CRYSTALLIZATION BEHAVIOR AND CRYSTALLOGRAPHIC PROPERTIES OF DL-ARABINOSE AND DL-XYLOSE DIASTEREOMER SUGARS

Bradley Tyson, Christopher M. Pask, Neil George, and Elena Simone*

Cryst. Growth Des. **2022**, *22*(2), 1371−1383 (Article)
DOI: 10.1021/acs.cgd.1c01329

RELATING CRYSTAL STRUCTURE TO SURFACE PROPERTIES: A STUDY ON QUERCETIN SOLID FORMS

Panayiotis Klitou, Ian Rosbottom, Vikram Karde, Jerry Y.Y. Heng, and Elena Simone*

Cryst. Growth Des. **2022**, *22*(10), 6103−6113 (Article)
DOI: 10.1021/acs.cgd.2c00707

Dr. Elena Simone. Photo courtesy of Elena Simone.

I am a chemical engineer by background who discovered the world of crystal engineering only recently. During my PhD I focused on the design of crystallization processes, with only little attention given to the crystal structure of the particle I was nucleating and growing. However, I soon realized that engineering crystal structures is critical to obtain particles with the correct physical and chemical properties. Hence, before designing processes I needed to learn how to design a crystal! Now I am leading my multidisciplinary group of engineers, chemists, and pharmacists, and we try to engineer simultaneously crystal structures and properties in order to produce particulate products with targeted attributes. We are working on food, pharmaceutical, and agrochemical materials, and it is amazing how similar and, at the same time, different these crystals are.

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RECENT ADVANCES IN NONCLASSICAL CRYSTALLIZATION: FUNDAMENTALS, APPLICATIONS, AND CHALLENGES

Haoyang Fu, Xing Gao, Xin Zhang, and Lan Ling*

Cryst. Growth Des. **2022**, *22*(2), 1476−1499 (Review)
DOI: 10.1021/acs.cgd.1c01084

Prof. Lan Ling. Photo courtesy of Lan Ling.

Nanoparticles such as metallic iron, iron oxides, colloidal particles, protein particles, bacteria, and cells in nature have special microstructures, functions, and specific active surfaces for pollutant migration, redox, catalysis, and stabilization. Surface engineering, nucleation, and growth of solids from solutions via surface reactions affect many natural processes and are fundamental for applications in pollution control and remediation. Therefore, it is an important basic scientific issue in environmental chemistry to study the interfacial interaction of pollutants and the corresponding microscopic changes on a single nanoparticle caused by the valence, microscopic bonding, interface distortion and stress of the interface, etc. Our research focuses on developing in situ and cryoelectron microscopy to uncover the secrets of surface and solid phase reactions of pollution control. For the first time, we have engineered the fine structure of nanocrystalline iron nanoparticles for the encapsulation of uranium. Atomically resolved 3D images of heavy metals at the interface between nanocrystalline metallic iron and iron oxide have been obtained without prior knowledge. Utilizing the D-band coordination effect of N and Fe in nitrogen-doped carbon supports, we designed the structure of iron-based bimetallic catalysts to optimize electron flow, chemical stability, and catalytic properties. We are working on engineering the crystallization of colloids with polymer-like contaminants in the nucleation stage for high-efficiency pollution control and resource recovery.

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ε-GA_2O_3 GROWN ON *c*-PLANE SAPPHIRE BY MOCVD WITH A MULTISTEP GROWTH PROCESS

Yu-Hsuan Hsu, Wan-Yu Wu, Kun-Lin Lin, Yu-Hsuan Chen, Yi-Hsin Lin, Po-Liang Liu, Ching-Lien Hsiao, and Ray-Hua Horng*

Cryst. Growth Des. **2022**, *22*(3), 1837−1845 (Article)
DOI: 10.1021/acs.cgd.1c01395

Prof. Ray-Hua Horng. Photo courtesy of Ray-Hua Horng.

I am Ray Hua Horng, affiliated with National Yang Ming Chia Tung University. My current research focuses on the development of wide bandgap oxide materials using MOCVD. I am particularly fascinated by the growth of novel single crystal materials, specifically for the next generation of wide bandgap oxide materials. While GaN and SiC materials have already reached a high level of maturity and are widely used, I am interested in exploring alternative materials that can potentially replace them.

However, I am aware that growing Ga_2O_3 presents significant challenges, especially when attempting to grow it on a sapphire substrate. Another hurdle is the growth of p-type Ga_2O_3, which poses its own set of challenges. Despite these difficulties, I believe it is worthwhile to address these problems and explore potential solutions. Overcoming these challenges would contribute significantly to the field and its advancements.

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REDUCING THE ELECTRON DELOCALIZATION OF FOX-7 TOWARD A THERMALLY STABLE EXPLOSIVE AS A HEXANITROSILBENE (HNS) REPLACEMENT

Zhaoyang Yin, Wei Huang*, Zhiwei Zeng, Yuji Liu, and Yongxing Tang*

Cryst. Growth Des. **2022**, *22*(3), 1867−1873 (Article)
DOI: 10.1021/acs.cgd.1c01411

Dr. Wei Huang. Photo courtesy of Wei Huang.

Crystal engineering is a very important topic for materials, especially for energetic materials. The configuration and stacking method of crystals have a very direct impact on the energy, thermal stability, and mechanical sensitivity of energetic materials. However, the control of the crystal of energetic materials is still in the blind exploration stage. Therefore, "how can ideal crystals be obtained through theoretical and traceable molecular design?", "what crystallization methods can be used to obtain ideal crystals?", and "how can good crystal quality still be obtained in mass production?" are the most important topics in crystal engineering about energetic materials in the future.

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DESIGN, GROWTH, AND CHARACTERIZATION OF CRYSTALLINE COPPER OXIDE P-TYPE TRANSPARENT SEMICONDUCTIVE THIN FILMS WITH FIGURES OF MERIT SUITABLE FOR THEIR INCORPORATION INTO TRANSLUCENT DEVICES

Maria del Pilar Aguilar del Valle, Luis Fernando Garrido, Juan Carlos Alonso-Huitrón, Luis augusto Terrones Pacheco, Héctor Cruz-Manjarrez, Jose Reyes-Gasga, Ana Laura Pérez-Martínez, and Arturo Rodríguez-Gómez*

Cryst. Growth Des. **2022**, *22*(4), 2168−2180 (Article)
DOI: 10.1021/acs.cgd.1c01243

As a researcher in crystal engineering, my journey has been filled with challenges and successes that have greatly impacted my career and personal growth. One of the biggest lessons I've learned is that perseverance and dedication are essential to succeeding in academia. Collaborations with colleagues, students, advisors, and mentors provide valuable insights, feedback, and guidance during the process of designing, growing, and characterizing crystalline thin films. The exchange of ideas through conferences, workshops, and seminars also promotes intellectual discussions and innovation. In developing copper oxide p-type transparent semiconductive thin films, I faced various difficulties ranging from material synthesis to film deposition. However, these challenges proved to be opportunities for learning and growth as I explored alternative techniques and methods. Through innovative approaches such as modifying growth parameters and implementing postdeposition treatments, I was able to achieve figures of merit suitable for incorporation into translucent devices. Overall, my experience as a researcher in crystal engineering has taught me the importance of collaboration, persistence, and resourcefulness in achieving success. It has also shown me how advances in materials science can contribute toward the development of novel technologies with significant impact on society.

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DIARYLIODONIUM TETRACYANIDOMETALLATES SELF-ASSEMBLE INTO HALOGEN-BONDED SQUARE-LIKE ARRAYS

Vitalii V. Suslonov, Natalia S. Soldatova, Pavel S. Postnikov, Giuseppe Resnati, Vadim Yu. Kukushkin, Daniil M. Ivanov*, and Nadezhda A. Bokach*

Cryst. Growth Des. **2022**, *22*(4), 2749−2758 (Article)
DOI: 10.1021/acs.cgd.2c00175

THERMODYNAMIC ANALYSIS OF HYBRID CHEMICAL VAPOR DEPOSITION OF TRANSITION-METAL-ALLOYED GROUP-III-NITRIDE SCALN PIEZOELECTRIC SEMICONDUCTOR FILMS

Mina Moradnia, Sara Pouladi, Jie Chen, Nam-In Kim, Onosetale Aigbe, and Jae-Hyun Ryou*

Cryst. Growth Des. **2022,** 22 (4), 2239−2247 (Article)
DOI: 10.1021/acs.cgd.1c01331

Mina Moradnia. Photo courtesy of Meysam Hariri.

Sara Pouladi. Photo courtesy of Meysam Hariri.

We have developed a new synthesis method that has the capability to grow high-quality piezoelectric films from III-N materials containing transition metal alloys to compete against commonly used hazardous PZT. Our growth technique allows for precise control over the material's composition, crucial in improving the final product's quality. This breakthrough could lead to great innovations in wireless communication and sensor technologies.

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GIANT SUPRAMOLECULAR SYNTHONS VIA CYCLIC HALOGEN···HALOGEN CONTACTS IN SUBSTITUTED *O*-XYLENES

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Cryst. Growth Des. **2022**, *22*(4), 2318−2327 (Article)
DOI: 10.1021/acs.cgd.1c01397

Dr. Nanditha Nair. Photo courtesy of Nanditha Nair.

My fascination for crystal engineering comes from my research background in synthetic organic chemistry. Adhering to a green chemistry protocol, I always opt for crystallization over column chromatographic methods for purifying organic products. Although lots of crystals were generated in the lab during my PhD work, I never looked into the crystal engineering aspect of the work until my postdoctoral position at IISER-Thiruvananthapuram with Prof. Mahesh Hariharan. Every new beginning needs tremendous moral and physical support from various sources. I started crystal engineering as a mainstream work, with the encouragement from my mentor. Crystal engineering has given me an opportunity to find my space among researchers. It has opened a new direction to my research. I look forward to exploring noncovalent interactions in forming unique supramolecular assemblies and then designing materials for various applications.

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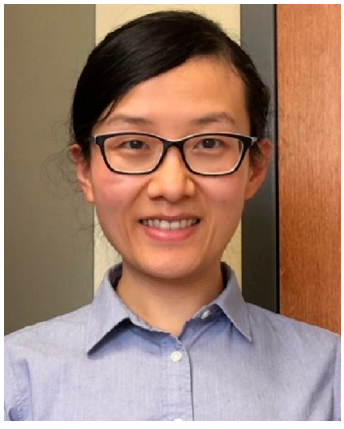
OUT WITH ACETONITRILE: WATER-ASSISTED ACCELERATED-AGING SYNTHESIS OF CuI-PYRAZINE HYBRID MATERIALS

Will A. Lucas and Feier Hou*

Cryst. Growth Des. **2022**, *22*(5), 3128−3137 (Article)
DOI: 10.1021/acs.cgd.2c00021



Dr. Feier Hou. Photo courtesy of Feier Hou.

As a researcher in crystal engineering, over the years, I have met many supportive mentors and colleagues in the field that greatly helped me with my career advancement. Having a supportive network is very important: not only can people help you with professional development such as writing letters of

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recommendation, but they can also help you get through difficulties you are experiencing by offering you support and/or helpful resources. For that reason, I strive to be part of the supportive network for my colleagues and students as well. As a faculty member, I strive to create a supportive and welcoming environment for all my students to help them succeed in achieving their personal and professional goals. I believe that when we work collaboratively and lift each other up, the future of the field will be bright.

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DESIGNING A HIGH-CRYSTALLINITY NANO-GAPPED PARTICLE SUPERLATTICE VIA DNA-GUIDED COLLOIDAL CRYSTALLIZATION AND DEHYDRATION

Hayato Sumi, Noboru Ohta, Hiroshi Sekiguchi, Shunta Harada, Toru Ujihara, Katsuo Tsukamoto, and Miho Tagawa*
Cryst. Growth Des. **2022**, *22*(6), 3708−3718 (Article)
DOI: 10.1021/acs.cgd.2c00075

Prof. Miho Tagawa. Photo courtesy of Miho Tagawa.

My research focuses on DNA-programmable nanoparticle self-assembly and crystallization. The turning point for me came 10 years ago when I joined the laboratory of Professor Ujihara, a specialist in semiconductor crystal growth, as an associate professor. Adding the perspective of colloidal crystal growth to the field of DNA nanotechnology, we have succeeded in assembling single crystals of well-designed, high-quality, large nanoparticle superlattices.

In Nagoya, I experienced childbirth alone and have been raising two children alone for 10 years. There are few opportunities for a couple of researchers to find jobs in the same area, and my husband lives separately as he works in a research institute far away. Furthermore, from 2019, solo parenting became very difficult due to extended school closures and frequent class closures for children due to COVID-19. I thought my career as a researcher was over. In the midst of these difficulties, I gathered my strength and wrote CGD papers.

Miho Tagawa
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POLYMORPHISM IN GRISEOFULVIN: NEW STORY BETWEEN AN OLD DRUG AND POLYETHYLENE GLYCOL

Xiao Ou, Shuting Li, Yunyun Chen, Haowei Rong, Ao Li, and Ming Lu*
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Prof. Ming Lu. Photo courtesy of Ming Lu.

In the very beginning, my lab focused on hot-melt extrusion for the manufacture of amorphous solid dispersions to enhance the dissolution of water-insoluble drugs. My interest in melt crystallization of small organic molecules started in the fall of 2015, when I measured the melting points of a series of drugs using solid dispersion technology and observed an unexpected phase conversion in vemurafenib, a drug clinically used to treat melanoma. As I began to explore the crystallization behavior of this drug, the beautiful spherulites and fantastic phase transformations between polymorphs caught my attention. That is a fascinating microworld! Following the publication of vemurafenib's polymorphism, we discovered a rich polymorph of nicotinamide, a derivate of vitamin B3. A strong desire to understand the crystal structure of these lovely spherulites drove me to develop the microdroplet strategy for growing single crystals from melts. For polymorphs that cannot be grown into single crystals with sufficient size, we cooperated with Dr. Hongyi Xu and Prof. Xiaodong Zou to use 3-D electron diffraction for structure elucidation. Thanks to these powerful methods, I freely enjoy exploring the beautiful and interesting world of crystals with my students and collaborators to understand nucleation, crystal growth, and polymorphic selectivity in melt crystallization.

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SYNTHESIS, STRUCTURE, AND TUNABILITY OF ZERO-DIMENSIONAL ORGANIC-INORGANIC METAL HALIDES UTILIZING THE *m*-XYLYLENEDIAMMONIUM CATION: MXD_2PbI_6, $MXDBiI_5$, AND $MXD_3Bi_2Br_{12}\cdot 2H_2O$

Pia S. Klee, Yuri Hirano, David B. Cordes, Alexandra M. Z. Slawin, and Julia L. Payne*
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Dr. Julia Payne. Photo courtesy of Julia Payne.

Research in my group focuses on materials for energy applications. We're particularly interested in how crystal structures influence the properties of materials which can be used in batteries of photovoltaics. Working in academia requires dedication, resilience, and curiosity. One tip I'd give to younger researchers is that a love of reading is also required to keep up to date with the literature! Building networks with researchers with skills complementary to your own is also really important.

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HIGH-MOBILITY MOCVD β-Ga_2O_3 EPITAXY WITH FAST GROWTH RATE USING TRIMETHYLGALLIUM

Lingyu Meng*, Zixuan Feng, A F M Anhar Uddin Bhuiyan, and Hongping Zhao*

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PULSED-MODE MOCVD GROWTH OF ZnSn(Ga)N_2 AND DETERMINATION OF THE VALENCE BAND OFFSET WITH GaN

Kaitian Zhang, Chenxi Hu, A. F. M. Anhar Uddin Bhuiyan, Menglin Zhu, Vijay Gopal Thirupakuzi Vangipuram, Md Rezaul Karim, Benthara Hewage Dinushi Jayatunga, Jinwoo Hwang, Kathleen Kash, and Hongping Zhao*

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I started to do research in the area of III-nitrides crystal epitaxy and device fabrication when I was a PhD student back in 2007. When I completed my PhD in 2011 and continued my professional career in academia, I expanded my research focus toward new semiconductors including II−IV-nitrides and Ga(In, Al)O for both optoelectronics and power electronics. Along my journey as a researcher, I consider myself fortunate to receive strong support from my PhD advisor Prof. Nelson Tansu and many pioneers in the field. I believe it is essential to build a more diverse and inclusive research community that will benefit society.

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ORIGINS AND IMPLICATIONS OF EXTRAORDINARILY SOFT CRYSTALS IN A FIXED-DOSE COMBINATION HEPATITIS C REGIMEN

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Dr. Rajni Miglani Bhardwaj. Photo courtesy of Rajni Miglani Bhardwaj.

Crystal engineering is a bottom-up technique to design and manufacture functional materials from molecular building blocks. In addition to particle engineering and formulation, it is one of the commonly used approaches to modulate the solid-state properties of active pharmaceutical ingredients to produce a drug product with desirable traits. From my experience, a deeper understanding of the structure−property relationships, i.e., molecular features, intermolecular interactions, and their consequences for the properties, is extremely valuable in designing better controlled pharmaceutical processes. Irrespective of the great success achieved via crystal engineering approaches, it is not always possible to obtain a predicted outcome based purely on assembly of these building blocks. While we may be able to obtain new solid forms with specific intermolecular interactions, their thermodynamic stability is not always ensured. Additionally, the experiments to obtain designed solid forms remain majorly empirical. The recent advancements in computational and analytical techniques are catalyzing deep research across academia and industry, and we need to build upon our strong foundations in making inroads into these challenges. I look forward to making a more meaningful impact of the understanding, development, and implementation of solid-state interventions via crystal engineering to higher quality drug substances and products.

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MBE-GROWN HYBRID AXIAL CORE−SHELL N−I−P GAASSB HETEROJUNCTION ENSEMBLE NANOWIRE-BASED NEAR-INFRARED PHOTODETECTORS UP TO 1.5 μm

Priyanka Ramaswamy, Kendall Dawkins, Hirandeep Kuchoor, Rabin Pokharel, Jia Li, and Shanthi Iyer*

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DOI: 10.1021/acs.cgd.2c00652

Dr. Priyanka Ramaswamy. Photo courtesy of Priyanka Ramaswamy.

My experience as a researcher in the semiconductor field was surreal, which I will cherish forever. As Richard Feynman said, there is definitely plenty of room at the bottom, and those tiny little nanowires prove that nothing is impossible. The valuable life lesson taught by the nanowire is just like how a catalyst is important for the growth of nanowires mentors play a crucial role in our personal and professional growth, so choose the right catalyst/ambience for your growth. That being said, I was/am fortunate to have supportive mentors throughout my life at NIT-Trichy, NCAT-Greensboro, and Micron Technology, who have encouraged me to approach even the negative results with a positive attitude. From my experience as a researcher, I would like to share that it is completely fine to fail/fall, but always make sure that you bounce back! Never Ever Give Up!

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Dr. Shanthi Iyer. Photo courtesy of Shanthi Iyer.

Worklife Balance: Worklife balance forced on women in motherhood provides an edge over others due to the inherent requirement of prioritizing, organizing, and maintaining flexibility.

Step Outside the Box: Being singled out as the only female faculty member for many years pushed me out of my comfort zone but allowed me to bring a different perspective or creative approach to the table due to my unique positioning.

Without a shadow of a doubt, we are making progress and moving in the right direction where women do not have to give 200% over others to prove our value.

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PROJECTED COST OF GALLIUM OXIDE WAFERS FROM EDGE-DEFINED FILM-FED CRYSTAL GROWTH

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As a non-PhD participant on projects, I bring a unique perspective directly informed by my years of manufacturing experience. I collaborate with researchers to understand technoeconomic trade-offs of early stage research. As an analyst, I help put research problems in context and analytically show technology potential through supply chain analysis, trade-flow mapping, market research, and bottom-up cost modeling. Working at a national lab is a unique juxtaposition of academia and industry. Often the challenge is having academics take seriously the need to show real world viability, while not have an *h*-index commiserate with that of top researchers. However, the support and encouragement of the colleagues I work with help overcome this hurdle. The biggest lessons I have learned are that curiosity overcomes lack of specific knowledge and diversity and new perspectives are critical to helping develop and advance the technology that will address hurdles to reaching a clean energy future.

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HETEROMETALLIC {FE18M6} (M = Y, Gd, Dy) PIVALATE WHEELS DISPLAY SOLVENT-INDUCED POLYMORPHISM

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Dr. Svetlana Baca. Photo courtesy of Svetlana Baca.

We are often faced with the choice of how to design new molecular crystalline solids with a predictable structure and specific physical and chemical properties. What preliminary building blocks should be included in the reaction mixture, and which ones are required? How will these building blocks interact with each other? How will they be connected in the final structure, and in what way? Is it possible to assemble the building blocks into crystalline materials of the desired topology and with a fixed chemical composition? In this case, knowledge and understanding of the principles of crystal engineering are crucial since all these issues can be addressed through crystal engineering studies.

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(111) FACETED METAL OXIDES: A REVIEW OF SYNTHETIC METHODS

Raiven I. Balderas, Cristian V. Ciobanu, and Ryan M. Richards*
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DOI: 10.1021/acs.cgd.2c00409

Ms. Raiven Balderas. Photo courtesy of Raiven Balderas.

Throughout my graduate career, one thing I have come to learn is that success and growth in all facets of life are the result of trial and error. Synthesizing (111) faceted metal oxides was an early task of mine that was accompanied by a myriad of failed attempts, but nonetheless one that I perfected with meticulous care and determination. And so, it is important to convey that within the constant error that may plague some research projects, there is always something to learn. I believe this concept is important to destigmatize because research is not always linear. There will be ups, downs, and sometimes unexpected results, but remaining optimistic and digging deeper for solutions are paramount. For that I am extremely grateful to the chemistry department at Colorado School of Mines, but more specifically to my advisor, Dr. Ryan M. Richards, who has always been available to answer my questions, bounce off ideas, have fruitful discussions, and catalyze my growth as a female scientist.

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EFFECT OF HOMOLOGATION ON THE POLYMORPHISM OF ANTHRANILIC ACIDS

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Crystal engineering involves designing and synthesizing new materials with specific properties through an understanding of the molecular and supramolecular interactions that govern their behavior. To excel in this field, a strong foundation in both chemistry and crystallography is essential, along with a passion for exploring universal principles and the perseverance to unravel exceptions. Success requires a deep appreciation of the complex interplay between structure, bonding, and function at the molecular level, as well as critical thinking, problem-solving, and communication skills. Additionally, building a supportive community of colleagues, mentors, and collaborators can provide valuable guidance, feedback, and opportunities for growth. As the field evolves rapidly, keeping up with the latest research and technological advancements is crucial. Thus, one must remain curious, inquisitive, and committed to lifelong learning to keep pace with this exciting and dynamic field.

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During my postgraduate education, I studied and engaged in crystallography, such as polymorphism research and cocrystal research. I have published two SCI articles as first author or cofirst author in 2022. Through this learning journey, I have a deeper understanding of the charm of crystallography. Crystal engineering is described as the design synthesis of functional crystalline substances and consists of many different operations, including the determination of the crystal structure, the use of this understanding when attempting to design a specific type of crystal structure, and finally the realization of the desired crystal properties. Through a variety of crystal engineering strategies, scientists and entrepreneurs design and manufacture a wide variety of crystalline materials and drugs with different functions to meet people's specific needs. At the same time, we believe that the future development of crystal engineering will be more rapid and high quality quantitative.

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METAL−ORGANIC FRAMEWORKS BASED ON A JANUS-HEAD BIQUINOLINE LIGAND AS CATALYSTS IN THE TRANSFORMATION OF CARBONYL COMPOUNDS INTO CYANOHYDRINS AND ALCOHOLS

Juana M. Pérez, Samuel Morales-Cámara, Francisco M. García-Salas, Noelia Ruiz-Cuevas, Mireya E. López-Vargas, Duane Choquesillo-Lazarte, Javier Cepeda, Jose A. García, Víctor Karim Abdelkader-Fernández, Antonio Rodríguez-Diéguez, Sara Rojas*, and Ignacio Fernández*
Cryst. Growth Des. **2022**, *22*(12), 7395−7404 (Article)
DOI: 10.1021/acs.cgd.2c00985

Dr. Sara Rojas obtained her PhD from the University of Granada (in 2014) with a work focus on the synthesis of porous materials and their application as drug delivery systems. After

finishing her PhD, she continued her studies at the Institute Lavoisier in Versailles (France, 2016) and the IMDEA Energy institute (Spain, 2018) under a framework of a Marie Curie Individual Fellowship and Atracción del Talento grant, respectively. In 2021, she joined the Biochemistry and Electronics as Sensing Technologies group thanks to a Juan de la Cierva Incorporación grant, and in 2022 she started her Ramón y Cjala contract. Her research focus is on the development of porous materials for biomedical and environmental applications.

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CATIONIC METAL−ORGANIC FRAMEWORKS SYNTHESIZED FROM CYCLOTETRAPHOSPHAZENE LINKERS WITH FLEXIBLE TENTACLES

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Cryst. Growth Des. **2022,** *22*(12), 7123−7132 (Article)
DOI: 10.1021/acs.cgd.2c00806

I was very excited when I heard "women in crystallography". The majority of my academic studies are related to crystal structures and coordination polymers. If you work in this field, crystallography is indispensable for you. Crystallography and related programs, for example olex, mercury, and platon, are very important to determine to the dimension of crystal structures and to characterize their supramolecular interactions. For this reason, I try to constantly improve myself in crystallography.

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SINGLE-CRYSTAL HYBRID LEAD HALIDE PEROVSKITES: GROWTH, PROPERTIES, AND DEVICE INTEGRATION FOR SOLAR CELL APPLICATION

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Ms. Ramya Krishna Battula. Photo courtesy of Ramya Krishna Battula.

As an experimental researcher in crystal engineering for solar energy harvesting materials, I found the field exciting and sometimes quite challenging. It took me months and years of persistent practice to get a good hold on the growth and characterization techniques, and I'm still on the learning curve. Theory helps understand the concepts, but the experimental part is a different story and requires lots of patience. Presenting my research at conferences, doctoral review meetings, and discussions with my research group, collaborators, etc. has given me a new perspective that helped me solve a few critical issues. Hence, feedback from the research community helps look at the same problem from a different angle and even solve it sometimes. The future of crystal engineering looks bright with applications in diverse fields such as pharmaceuticals, polymers, smart materials, solar energy harvesting materials, etc., and it would give me joy and success to continue being a small part of it.

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SHEAR-INDUCED CRYSTALLIZATION AND RHEOLOGICAL ANALYSIS OF A THERAPEUTIC PROTEIN

Joana Ferreira*, João Carneiro, and João Moreira de Campos

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DOI: 10.1021/acs.cgd.2c00557

Dr. Joana Ferreira. Photo courtesy of Joana Ferreira.

My research interests in crystal engineering rely on multidisciplinary perspectives to solve problems through the combination of experimental, numerical, and analytical approaches. Although protein crystallization has been known since 1840, most of the bottlenecks found over the last 180 years cannot be solved nowadays. This intriguing dilemma has motivated me throughout my PhD project and still nowadays during my postdoctoral adventure. Scientific collaboration and networking have been playing a crucial role during my young research career, not only in terms of the acquired technical knowledge through scientific dissemination but also the involvement with the scientific community. This last aspect is continuously supporting me to deal with failure and succeed in this research field. I aim to increase my standing and influence in the scientific community, thus enhancing my prospects of building my own research group within 5−10 years at a leading institution.

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Cryst. Growth Des. 2023, 23, 3917−3930

INVESTIGATION ON THE MICROSTRUCTURES AND MECHANICAL PROPERTIES OF THE SHELLS OF *TRIDACNA CROCEA*

Baosheng Li, Ningjing Song, Yue Su, Jiangfeng Li, Ercai Pan, Chenxu Wang, Juan Gao, and Yurong Ma*

Cryst. Growth Des. **2022**, *22*(12), 6903−6916 (Article)
DOI: 10.1021/acs.cgd.2c00530

Prof. Yurong Ma. Photo courtesy of Yurong Ma.

Yurong Ma completed her Ph.D. in physical chemistry from Peking University, China, in 2004. She then went to the Max Planck Institute of Colloids and Interfaces, Germany, to work on nonclassical crystallization processes. Later, she worked on biomineralization at the Weizmann Institute of Science, Israel. Now she is working at the School of Chemistry and Chemical Engineering, Beijing Institute of Technology, China. Yurong Ma's research field is biomineralization and bioinspired crystallization. Her lab studies the relation between the (hierarchical) structure and functional property of biominerals, biomimetic crystallization, and bioinspired composite materials. Her research interests include the nucleation, crystallization, and crystal alignment control of inorganic and organic nanocomposites.

Yurong Ma
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PHARMACEUTICAL SALTS OF PIROXICAM AND MELOXICAM WITH ORGANIC COUNTERIONS

Shan Huang, Dean S. Venables, and Simon E. Lawrence*

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Miss Shan Huang. Photo courtesy of Shan Huang.

Being a researcher in crystal engineering can be a rewarding but challenging experience. It is a science and also a practical process that requires both scientific methods and artistic perception. On a daily basis, I utilize my knowledge of physics, chemistry, and mathematics, along with various tools and techniques like X-ray diffraction, thermal analysis, and infrared spectroscopy, to examine the structures and characteristics of crystals. I find a great sense of accomplishment and satisfaction when I am able to modify the physicochemical and biopharmaceutical properties of drug molecules by exploring their crystalline forms. Meanwhile, what I find particularly enjoyable is using aesthetic and artistic perspectives to observe the beauty and wonder of crystals. The shape, color, and texture of crystals can bring visual enjoyment to people and can also inspire me to discover some special properties of crystals, which is also the charm of crystal engineering.

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AN ANALYSIS OF PUBLICLY AVAILABLE MICROGRAVITY CRYSTALLIZATION DATA: EMERGENT THEMES ACROSS CRYSTAL TYPES

Hannah Wright, Amari Williams, Ashley Wilkinson, Lynn Harper, Ken Savin, and Anne M. Wilson*

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Prof. Anne Wilson. Photo courtesy of Anne Wilson.

After a semester sabbatical investigating the literature for crystal data and a summer of full-time work, my undergraduate research students and I were able to identify that the microgravity environment enhanced crystal growth across a diverse set of experiments and positively impacted all identified metrics. After completing our initial survey, we have been engaged in following up our study and are currently exploring a deeper dive into microgravity crystallization conditions. While this area is new to me, it was gratifying to engage with a supportive community that appreciates me and my students' novice perspective.

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CRYSTAL PHASE, ELECTRONIC STRUCTURE, AND SURFACE BAND BENDING OF $(In_xGa_{1-x})_2O_3$ ALLOY WIDE-BAND-GAP SEMICONDUCTORS

Zhenni Yang, Wenshan Chen, Siliang Kuang, Ziqian Sheng, Jueli Shi, Duanyang Chen, Meiyan Cui, Hongji Qi*, and Kelvin H. L. Zhang*

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Miss Zhenni Yang. Photo courtesy of Zhenni Yang.

I'm Zhenni Yang, a PhD candidate at the College of Chemistry and Chemical Engineering, Xiamen University under the supervision of Prof. Kelvin H. L. Zhang. As a researcher in crystal engineering, my research interests focus on the epitaxial growth of wide bandgap oxide semiconductor thin films such as Ga_2O_3 and In_2O_3 using pulsed laser deposition. I'm dedicated to regulating the optical and electrical properties of semiconductor crystals by doping or alloy engineering for various device applications and analyzing the relationship between crystal electronic structures and device performances by combining photoelectron spectroscopy and density functional theory calculation. For me, curiosity and patience are incredibly important parts of the scientific process, which encourage me to face failure and never give up. What's more, the collision of ideas often leads to new inspiration. Discussing with partners will often make you get twice the result with half the effort.

Zhenni Yang
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WOMEN RESEARCHERS AT THE FOREFRONT OF CRYSTAL ENGINEERING

We thank all the women researchers at the forefront of crystal engineering who contributed to this profile and virtual issue.

Sonja Krane, Senior Associate Publisher, American Chemical Society orcid.org/0000-0002-6525-8067

Jennifer Hiscock, Professor of Supramolecular Chemistry, University of Kent, Chair (2019−2023) and Advisory Board Chair (2023−onwards), Women in Supramolecular Chemistry Network; Chair (202−onwards), Royal Society of Chemistry Macrocyclic and Supramolecular Chemistry (MASC) interest group (United Kingdom) orcid.org/0000-0002-1406-8802

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Notes

Views expressed in this editorial are those of the authors and not necessarily the views of the ACS.

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