Information & Agenda

Scoping Workshop

Programme Book

Hannover, Germany | 27- 29th November 2024

NANOCONFINEMENT IN CHEMISTRY

TINKERING WITH NANOPOROUS ARCHITECTURES TO SOLVE CONTEMPORARY SOCIETAL ISSUES

Supported by

VolkswagenStiftung

Welcome
to the Scoping Workshop

Nanoconfinement in Chemistry

In recent years, advances in the chemistry of porous systems have opened exciting new avenues for both fundamental research and practical applications. Nanoporous materials, with their unique ability to confine molecules within spatially restricted environments, offer remarkable opportunities to manipulate chemical reactions, enhance selectivity, and tailor material properties. This confinement often brings about an emergent and unexpected behavior, highly influenced by surfaces and governed by thermodynamic principles that differ from those observed in bulk systems, leading to novel insights into reaction dynamics, phase transitions, and molecular interactions at the nanoscale.

As we continue to refine our understanding of confinement effects, the potential for porous materials in industrial and applied settings becomes increasingly clear. From catalysis and energy storage to sensing and environmental remediation, nanoporous architectures are being integrated into cutting-edge devices and technologies designed to tackle some of the most pressing societal issues. These systems not only optimize chemical processes but also contribute to more sustainable solutions in diverse fields.

On the other hand, many aspects of confinement remain unexplored and are far from being fully understood or effectively applied in material fabrication and applications. Characterization techniques still encounter limitations at small length scales and rapid time intervals. Modeling, which is crucial for resolving these fine scales, has recently seen rapid advancements, particularly with the integration of artificial intelligence. Together, these developments offer exciting prospects for fundamental research and innovative technologies, addressing the future challenges facing our society.

This workshop will delve into the latest advancements in nanoconfinement, exploring how the interplay among disciplines - ranging from material synthesis, characterization, and modeling to technological applications - can be harnessed to help address today's societal challenges. We aim to foster interdisciplinary discussions that inspire new strategies and collaborations for the development and application of nanoconfinement, thereby establishing a nucleus for a community dedicated to tackling future challenges across academia and industry using the powerful concepts developed at tiny scales.

Prof. Annette
Andrieu-Brunsen
TU-Darmstadt, Germany
Macromolecular Chemistry – Smart Membranes
Organiser

Prof. Omar
Azzaroni
INIFTA, La Plata, Argentina
Soft Matter Laboratory
Organiser

Prof. Galo
Soler-Illia
UNSAM, San-Martin, Argentina
Nanoarchitectures Lab
Organiser

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Venue Location

Where to go

Venue Address: Tagungszentrums Xplanatorium Herrenhausen
Herrenhäuser Straße 5, 30419 Hanover.

Key Locations

Conference Venue Xplanatorium Herrenhausen

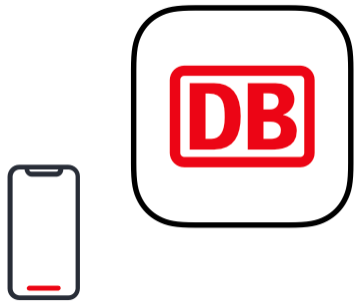
The tram stop closest to the venue, „Herrenhäuser Gärten“, can be reached from the hotel via the lines 4 and 5 in direction „Garbsen“ or „Stöcken“. Tickets for public tranportation will be available either in the hotel or at the workshop location.

Grand Hotel Mussmann

Hotel rooms for every participant are reserved for 3 nights (arrival Tuesday 26th, departure Friday 29th) at the Grand Hotel Mussmann, Ernst-August-Platz 7, 30159 Hannover. The station closest to the hotel is „Kröpcke“. Breakfast will be served in the hotel.

Hannover Airport

For those arriving by plane there is the option to take the train line S5 to the Hannover main station (Hauptbahnhof), the train station is located beneath terminal C and the ride takes approx. 20 min. Refer to the DB app for more details of the route.



Deutschbahn (DB) app

We recommended that you download this app which provides navigation, tickets and scheduling for buses and trains both in and around Hannover.

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Goals & Concept

The Workshop aims to encourage a **reflection and further development** of the interdisciplinary research area and community related to **nanoconfinement in chemistry – tinkering with nanoporous architectures to solve contemporary societal issues**. The **current status** of this field of research should be assessed and, on this basis, **perspectives for its further development** should be worked out. This may include the exchange about how this field of research is doing; what could be done differently in it; what potentials exist and how they could be realized; and how we can initiate developments. Thus, **discussion and intensive exchange** together with developing a **community** able and **willing to tackle the identified future perspectives ar**e at the core of our scoping workshop. This may include...

... identifying ways to establish or consolidate newly emerging research areas,
...an elaboration of strengths, weaknesses, and development of perspectives for an existing research area,
...an identification of intersections and cooperation potentials between different research areas,
...the development of strategic recommendations for actors in science policy, science funding or science management to support the further development of a research area.

The following Session Topics will structure our workshop:

- Session TOPIC 1: **Opening**
- Session TOPIC 2: **Material fabrication today and tomorrow**
- Session TOPIC 3: **Modeling: from explanation to predictive tools**
- Session TOPIC 4: **Confinement-derived properties**
- Session TOPIC 5: **(new) confinement-based technologies and social impact**

To achieve these goals each session will be structured into:

a) **Short impulse** presentations
b) **Small group discussions** at work stations to exchange and focus specific ideas
c) **Plenary discussion** to synthesize the small group discussions into a bigger picture& collect final input

All discussions will be documented by the participants as the discussion results will serve to write a **position paper** with all participants after the workshop. Summarizing the main results into a position paper is an essential part of the workshop.

Further information on this workshop format:
https://www.volkswagenstiftung.de/en/funding/funding-offer/scoping-workshops

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Workshop Participants

Overview

Prof. Markus ANTONIETTI

MPI für Kolloid- und Grenzflächenforschung, Germany
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Dr. Hikmat BINYAMINOV

MPI für Kolloid- und Grenzflächenforschung, Germany
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Prof. Lydéric BOCQUET

CNRS,
Collège de France
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Prof. Angela DANIL DE NAMOR

University of Surrey, UK
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Prof. Maria FYTA

RWTH Aachen, Germany
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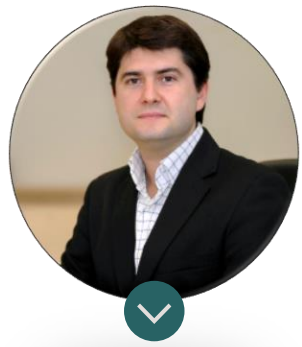
Prof. Javier GARCÍA-MARTÍNEZ



International Union of Pure and Applied Chemistry (IUPAC),
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Prof. Stefan **GULDIN**

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Prof. Stefan **HOWORKA**

University College London, UK
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Prof. Laurent **JOLY**

Université Lyon, France
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Dr. Christian **KUTTNER**

Editor, Nature Communications
christian.kuttner@nature.com

Dr. Stefan **LAMOTTE**

BASF, Deutschland
Stefan.Lamotte@basf.com

Prof. Serge **LEMAY**

Twente University, Mesa+ Institute, Netherlands
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Prof. Bettina **LOTSCH**

MPI für Festkörperfroschung, Stuttgart, Germany
b.lotsch@fkf.mpg.de

Prof. Shlomo **MAGDASSI**

Hebrew University of Jerusalem, Israel
Shlomo.Magdassi@mail.huji.ac.il

Prof. Kazuki **NAKANISHI**

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Dr. Carsten **PLUEG**

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Prof. Sebastian **POLARZ**

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Prof. Lilo **POZZO**

University of Washington, USA
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Dr. Matías **RAFTI**

University of La Plata, Argentina
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Prof. Matthias **REHAHN**

Technische Univeresität Darmstadt
Germany
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Dr. Anke G **ROTH**

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Prof. Clément **SANCHEZ**

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Prof. Damián **SCHERLIS**

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Prof. Igal **SZLEIFER**

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Prof. Matthias **THOMMES** Prof. Kristina **TSCHULIK**

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04

Moderation & Documentation

Overview

Hannes **SCHLENDER**

science RELATIONS
Moderation & Documentation

Dirk **HANS**

science RELATIONS
Moderation & Documentation

Lisa **BALONIER**

Technische Universität Darmstadt
Macromolecular Chemistry Smart Membranes
PhD Candidate
Documentation & Support

Michael **ZOPPELT**

Technische Universität Darmstadt
Macromolecular Chemistry - Smart Membranes
PhD Candidate
Documentation & Support

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Agenda

Day 1

Wednesday
November 27 | 2024

SR 4 | 08:30
Registration & Coffee

SR 4 | 09:00 – 12:30
Opening & Topic Reflection

SR 4 | 09:00
Welcome
Prof. Soler-Illia, Prof. Azzaroni, Prof. Andrieu-Brunsen

SR 4 | 09:30
Impulse Presentations:
Prof. Sanchez, Dr. Lamotte, Prof. Garcia-Martinez

SR 3 & 4 | 10:00
Small Group Discussions

S. Lamotte & G. Soler-Illia

J. Garcia-Martinez & A. Andrieu-Brunsen

C. Sanchez & O. Azzaroni

- Work station I : Reproducibility of silica supports: The key for validation of chromatographic applications
- Work station II : Embracing Complexity: Nanoengineering Confinement in Catalystic Materials for Previously Inaccessible Reactions.
- Work station III: How biomimetic can we get - pores / confinement as building block

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SR 4 | 11:15
Coffee Break
Light refreshments and snacks will be served

SR 4 | 11:30
Plenary Discussion
Prof. Sanchez, Dr. Lamotte, Prof. Garcia Martinez

Festsaal | 12:30 - 14:30
Lunch

Agenda
Day 1

Wednesday
November 27 | 2024

SR 4 | 14:30 - 18:00
Material Fabrication Today and Tomorrow

SR 4 | 14:30
Impulse Presentations:
Prof. Lotsch, Prof. Nakanishi, Prof. Magdassi

SR 3 & 4 | 15:00
Small Group Discussions
S. Magdassi & S. Polarz
B. Lotsch & M. Rafti
K. Nakanishi & A. Andrieu-Brunsen

work station I : New fabrication technologies such as additive manufacturing
work station II : Confinement-feature desing using nanobuilding blocks & data-driven synthesis
work station III: Integration of confined functions into multiple length scales

SR 4 | 17:00
Coffee Break
Light refreshments and snacks will be served

SR 4 | 17:30
Plenary discussion on topics
Prof. Lotsch, Prof. Nakanishi, Prof. Magdassi

Festsaal | 18:30
Dinner

20:00
Industry view on Future Challenges
Drinks & Networking
C. Plüg & A. Roth

21:45
Transfer to Hotel

Agenda
Day 2

Thursday
November 28 | 2024

SR 4 | 08:30
Welcome Coffee

SR 3 & 4 | 09:00 – 12:30
Modeling: from Explanation to Predictive Tools

SR 4 | 09:00
Impulse Presentations:

Prof. Joly, Prof. Scherlis, Prof. Szleifer

SR 3 & 4 | 09:30
Small Group Discussions

L. Joly & D. Scherlis
M. Rehahn & M. Fyta
I. Szleifer & G. Soler-Illia

- Work station I : How to manage complexity in pores: How predictive can we get?
- Work station II : ML/AI/ digital twins: hype or added value?
- Work station III: Theory of mimicking biopores - how biomimetic can we get?

SR 4 | 11:00
Coffee Break

Light refreshments and snacks will be served

SR 4 | 11:30
Plenary Discussion

Prof. Joly, Prof. Scherlis, Prof. Rehahn

Festsaal| 12:30 - 14:30
Lunch

Agenda
Day 2

Thursday
November 28 | 2024

SR 3 & 4 | 14:30 - 18:00
Confinement-derived Properties

SR 4 | 14:30
Impulse Presentations:
Prof. Thommes, Prof. Howorka, Prof. Guldin

SR 3 & 4 | 15:00
Small Group Discussions

M. Thommes & K. Tschulik
- work station I : (in-situ, in-operando, high resolution) characterization, difficulty in separating variables

S. Howorka & S. Lemay
- work station II : Nanofluidics, compartments and out of equilibrium systems

S. Guldin & H. Binyaminov
- work station III: New confinement-derived properties

SR 4 | 17:00
Coffee Break
Light refreshments and snacks will be served

SR 4 | 11:30
Plenary Discussion
Prof. Thommes, Prof. Howorka, Prof. Guldin

Festsaal | 18:30
Dinner

20:00
"From an Editor‘s Perspective: How Do We Evaluate Scientific Progress?“.
Dr. C. Kuttner

21:45
Transfer to Hotel

Agenda
Day 3

Friday
November 29 | 2024

SR 4 | 08:30
Welcome Coffee

SR 3 & 4 | 09:00 – 12:30
Confinement-based Technologies & Social Impact

SR 4 | 09:00
Impulse Presentations:

Prof. Antonietti, Prof. Bocquet, Prof. Danil de Namor , Prof. Pozzo

SR 3 & 4 | 09:30
Small Group Discussions

M Antonietti & O. Azzaroni
A. Danil de Narmor & A. Andrieu-Brunsen

L. Bocquet & L. Pozzo

- Work station I : New confinement-derived technology & Nanothermodynamics
- Work station II : Confinement based expected improvement / challenges in existing technology
- Work station III: New technology, pace of innovation, hurdles for innovation and solutions

SR 4 | 11:00
Coffee Break

Light refreshments and snacks will be served

SR 4 | 11:30
Plenary Discussion

Prof. Antonietti, Prof. Bocquet, Prof. Danil de Namor , Prof. Pozzo

Festsaal | 12:30 - 13:30
Lunch

Agenda
Day 3

Friday
November 29 | 2024

13:30
Final Wrap up
Was something missing for the position paper?

14:30
How to continue after the Workshop

15:00
Goodbye

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Biography

Prof. Annette Andrieu-Brunsen

Annette Andrieu-Brunsen studied Chemistry at the Philipps-Universität Marburg (Germany). She got her PhD from the Johannes-Gutenberg Universität and the Max-Planck-Institute for Polymer Research in Mainz (Germany) partly funded by the Studienstiftung des Deutschen Volkes in 2010 and has been working together with Prof. Soler-Illia and Prof. Azzaroni at the CNEA in Buenos Aires (Argentina) before being appointed as the Assistant Professor at the TU-Darmstadt (Germany). In 2018 he was appointed as an associate professor at TU-Darmstadt and in 2020 she was appointed as a full professor at TU Darmstadt (Germany). She received several awards and was granted an ERC StG in 2018. Her research interest focuses on functional nanopore and nanopore transport design. This includes polymer function-alization of spatially confined nanopores, nanopore wetting and charge control, innovative nanoporous material and architecture design as well as automated design procedures.

Prof. Markus Antonietti

Markus Antonietti is Director for “Colloid Chemistry” at the Max Planck Institute of Colloids and Interfaces and Full Professor at the University of Potsdam (Germany).

Biography

Prof. Omar Azzaroni

Omar Azzaroni is a chemist who earned his PhD from the Universidad Nacional de La Plata (UNLP) (Argentina) in 2004. He pursued postdoctoral research at the University of Cambridge (UK) as a Marie Curie Research Fellow (2004–2006) and at the Max Planck Institute for Polymer Research (Germany) as an Alexander von Humboldt Research Fellow (2007). From 2009 to 2013, he led a Max Planck Partner Group. He also served as Vice-Director of the Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA) from 2012 to 2015. Currently, he is a Senior Research Fellow at CONICET, leads the Soft Matter Laboratory at INIFTA, and is a Full Professor at UNLP. He is also a co-founder and scientific advisor of Gisens Biotech. His research expertise spans nanostructured hybrid interfaces, supramolecular and macromolecular materials science, and soft nanotechnology, with a focus on the integration of functional molecular systems into devices such as solid-state nanopores, graphene-based transistors, and bioelectrochemical sensors.

Dr. Hikmat Binyaminov

Dr. Hikmat Binyaminov did his PhD in Chemical Engineering at the University of Alberta in Canada. In thesis, titled Some Topics in Interfacial and Solution Thermodynamics, he has studied the interplay of geometry and thermodynamics in certain at small scale and multicomponent solutions. Currently he is a postdoc at the Max Planck Institute of Colloids and Interfaces working on Thermodynamics of Quantum-sized Systems with Prof. Antonietti.

Biography

Prof. Lydéric Bocquet

Prof. Lydéric Bocquet is Professor at CNRS and Professor of Physics at ENS Ecole Normale Supérieure, Paris (France).

Prof. Angela Danil De Namor

Professor Angela F Danil de Namor, PhD, DSc, FRSC, CChem, FMNAS (Argentina), IUPAC Fellow

Emeritus and Honorary Professor of Physical Chemistry (University of Surrey (UK), Dr Honoris Cause of three Universities in Latin America. Has published over 170 scientific publications and eight on international collaborations. Has given forty plenary and keynote lectures at international conferences. Has supervised over 50 students al PhD and over seventy at MSc levels. Further information in surrey.ac.uk/chemistry/people/danildenamor.

Biography

Prof. Maria Fyta

Maria Fyta has studied Physics in Greece, where she also obtained her PhD in Computational Condensed-Matter Physics in 2005. She had two postdoctoral stays in the USA and Harvard University (group of E. Kaxiras) and Germany at the Technical University of Munich (group of R.R. Netz) with a Marie Curie and a Humboldt fellowship. She was appointed a Juniorprofessor in Physics at the University of Stuttgart, Germany in 2012 and a Professor in Computational Biotechnology at the RWTH Aachen University, Germany in 2021. Her group is using computational tools at various spatiotemporal scales in order to model and understand intra- and inter-molecular interactions in diverse systems. Example of these are nanostructured and 2D heterostructures, nanopores, (bio)functionbalized templates, ionic solutions, and (bio)molecules related to biosensing, nanoelectronic, and catalytic applications.

Prof. Javier García-Martínez

Professor of Inorganic Chemistry and Director of the Molecular Nanotechnology Lab at the University of Alicante, Spain.

President of the International Union of Pure and Applied Chemistry (IUPAC) during the 2022-2023 biennium.

Founder of Rive Technology, the company that commercialises his catalysts, he started, grew and recently sold this business to Grace, the largest catalyst manufacturer.

This technology is now widely used in academic laboratories and chemical companies around the world, saving hundreds of thousands of tonnes of CO2 per year by reducing the amount of waste and coke that would otherwise be burned to produce green gas emissions in key industrial processes ranging from biomass conversion to catalytic cracking.

His contributions to catalysis, energy and chemistry have been recognised with some of the most prestigious awards, including the Kathryn C. Hach Award for Entrepreneurial Success by the American Chemical Society, he is Honorary Fellow of the Royal Society of Chemistry, and this year he got the National Research Award by the King of Spain

Biography

Prof. Stefan Guldin

Stefan Guldin, PhD CEng FHEA FIoP FRSC is Professor (Chair) of Complex Soft Matter at Technical University of Munich (since 2024). Currently, he is seconded to TUMCREATE, where he serves as Scientific CoDirector and Resident PI of the Proteins4Singapore project. SG studied physics at Karlsruhe Institute of Technology (2003-05) and the Technical University of Munich (2005-08) and graduated with a PhD from the University of Cambridge in 2012. After postdoctoral work at EPFL, he joined University College London in 2015 as lecturer and head of the Adaptive & Responsive Nanomaterials Lab and was subsequently promoted to associate (2018) and full professor (2022).

Prof. Stefan Howorka

Stefan Howorka is Professor of Chemical Biology at the Department of Chemistry at University College London (UCL). He obtained his PhD from the University of Vienna in 1999 and performed his postdoctoral research at Texas A&M University. After a 3-year stint at a biotech incubator, he joined UCL and was promoted to Professor in 2016. His research interests include the characterization of biological protein and peptide pores, the design of synthetic membrane nanopores composed of DNA for biosensing, and the development of DNA-based research tools for membrane biophysics (www.howorkalab.com). He has published 120 scientific papers including 25 in Nature X/Science, and is co-inventor on a protein pore technology used for portable and low-cost DNA sequencing.

Biography

Prof. Laurent Joly

Laurent Joly is a professor at the University of Lyon 1 - Institut Lumière Matière, specializing in molecular modeling of liquids at interfaces and in confined environments. His current research focuses on osmotic transport and interfacial friction, both from a fundamental perspective and with applications to the water-energy nexus.

Dr. Christian Kuttner

Christian Kuttner studied chemistry at the University of Bayreuth, Germany, and earned his PhD in 2014, focusing on macromolecular interfaces and colloidal materials. Afterward, he conducted postdoctoral research at the Leibniz Institute of Polymer Research (IPF) in Dresden, developing nanostructured materials with optical functionalities. In 2018, he joined Prof. Luis M. Liz-Marzán's group at CIC biomaGUNE, Spain, as a principle investigator within a Marie Skłodowska-Curie fellowship, continuing his work on nano-confined chemistry and optically functional materials. Since 2021, he has been an editor for Nature Communications, and in 2024, he was awarded the Bundestag Fellowship "Science meets Politics.

Dr. Christian Kuttner is a Senior Editor at Nature Communications and since 2021 responsible for physical chemistry content with a focus on nanomaterials. Before becoming a full-time editor, he conducted research as a Marie Skłodowska-Curie fellow at the CIC biomaGUNE in Donostia-San Sebastian, Spain, and as a postdoctoral researcher at the Leibniz Institute of Polymer Research (IPF) in Dresden, Germany.

Biography

Dr. Stefan Lamotte

Stefan Lamotte is an expert in separation science and a developer of new chromatographic techniques. He is a senior principal scientist in liquid chromatography at BASF and a lecturer at the Bonn/Rhein/Sieg University of Applied Sciences (HRBS) as well as co-author of several books and a well-recognized speaker with more than 100 poster & oral presentations at chromatography conferences and universities all over the world. Stefan Lamotte studied chemistry at the University of Saarland, Saarbrücken (Germany) where he was working with Prof. Engelhardt on stationary phases of fast HPLC during his PhD thesis in 1998. Stefan Lamotte was, among others, recognized as nominated member of the international scientific committee of International Symposium on High Performance Liquid Phase Separations and Related Techniques (HPLC 2027) in Innsbruck (Austria) and as Gerhard-Hesse-Award Winner of German Chemical Society, Working Party Separation Science. He currently is the vice president Working Party Separation Science of German Chemists Society (GDCh) and a member of the Working Party Chromatographic Separation Technologies (CST) expert group of European Pharmacopeia (PhEur) in Strasbourg.

Prof. Serge Lemay

Serge G. Lemay received a B.A.Sc. in Electrical Engineering with minor in Physics from the University of Waterloo, Canada, in 1993, and a Ph.D. in Physics from Cornell University, USA, in 1999. He was faculty at Delft University of Technology, The Netherlands, from 2001 to 2009. In 2009 he relocated to the University of Twente, The Netherlands, where he heads the Bioelectronics group, part of the Faculty of Science and Technology and the MESA+ Institute for Nanotechnology. His research has spanned solid-state physics (charge-density waves), molecular electronics (quantum effects in carbon nanotubes) and biophysics (DNA electrostatics). His main interests at present include the fundamentals of ion transport under confinement, and exploring digital transduction approaches in electrochemical nanofluidics.

Biography

Prof. Bettina Lotsch

Bettina is Director of the Nanochemistry Department at the Max Planck Institute for Solid State Research (MPI-FKF) in Stuttgart, Germany. She studied Chemistry at the Ludwig-Maximilians-Universität München (LMU) and the University of Oxford and received her PhD from LMU Munich in 2006. After a postdoctoral stay at the University of Toronto she became professor at LMU Munich in 2009 and was appointed Director at MPI-FKF in 2017. She also holds honorary professorships at LMU Munich and the University of Stuttgart, and is PI of the Munich-based Cluster of Excellence e-conversion.

Bettina's work has been recognized by a number of awards, including an ERC Starting Grant (2014) and the EU-40 Materials Prize of the EMRS (2017).

Prof. Shlomo Magdassi

Shlomo Magdassi is a professor at The Hebrew University of Jerusalem's Institute of Chemistry. His research centers on micro and nanomaterials, with a focus on their applications in functional 2D and 3D printing, printed electronics and soft robotics. Over the course of his career, he has published more than 360 papers, edited four books, and holds approximately 300 patents and applications. Besides publications, His research outcome includes the creation of numerous commercial activities, including start-up companies, licensing agreements, and worldwide sales. In recognition of his contributions, he was awarded the 2022 Johann Gutenberg Prize by the Society for Imaging Science and Technology, The Israel Chemical Society Award for Outstanding Scientist in 2024 , and he is also a Fellow of the National Academy of Inventors.

Biography

Prof. Kazuki Nakanishi

1986 Assistant Professor, Faculty of Engineering, Kyoto University

1995 Associate Professor, Graduate School of Engineering, Kyoto University

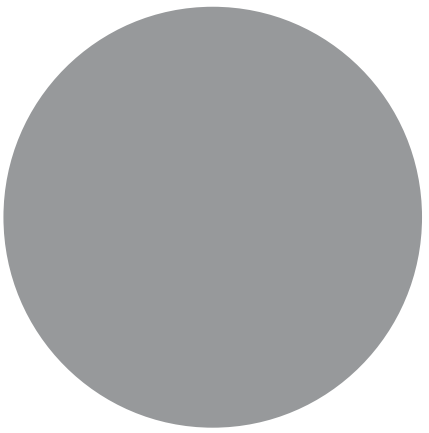
2005 Associate Professor, Graduate School of Science, Kyoto University

2019 Full Professor, Institute of Materials and Systems for Sustainability, Nagoya University

2019 Project-specific Professor, Institute for Cell-Materials Sciences, Kyoto University

Started working at Faculty of Engineering, Kyoto University in 1986, and obtained Doctor of Engineering degree in 1991. Received D.R. Ulrich Award from International Sol-Gel Society, ISGS, (1997), Gottardi Prize from International Commission on Glass (1999) and ISGS Life Achievement Award (2022). Stayed in Johannes Gutenberg University, Mainz (2000) and University of Montpellier II (2011) as Guest Professor. Currently President of Japanese Sol-Gel Society since 2019, Co-editor of Journal of Sol-Gel Science and Technology since 2009, fellows of Japanese Ceramic Society and International Sol-Gel Society since 2019. Main research interest is “Solution-based structural design of porous materials”, ~350 peer reviewed publications with ~21000 total citations (h-index: 74).

Dr. Carsten Plueg



Dr. Carsten Plueg is Global Head Innovation & Application Surface Solutions at MERCK (Darmstadt, Germany).

Biography

Prof. Sebastian Polarz

Sebastian Polarz is currently the chair for Inorganic Chemistry: Molecular and Material Science at Leibniz University in Hannover. His research is focused on semiconductor nanostructures for applications in optics, as well as nanoporous organosilica materials for new applications in water treatment and added-value surfactants. He studied chemistry at the University of Bielefeld. In 2001 he finished his Doctorate in the group of Prof. Antonietti at the Max-Planck Institute of Colloids and Interfaces in Potsdam. In the same Year Sebastian Polarz received the Otto-Hahn Award of the Max-Planck Society. In 2007 he became a professor of solid-state chemistry at the University of Konstanz.

Prof. Lilo Pozzo

Prof. Pozzo's research interests are in the area of colloids, polymers and soft-matter systems. Her research group focuses on controlling and manipulating materials structure for applications in healthcare, alternative energy and sustainability. Her group also develops and utilizes laboratory automation and artificial intelligence (AI) to accelerate the development time-scales of new materials and applies advanced techniques based on neutron and x-ray scattering to characterize their nanostructure. Prof. Pozzo obtained her B.S. from the University of Puerto Rico at Mayagüez and her PhD in Chemical Engineering from Carnegie Mellon University in Pittsburgh PA. She also worked at the NIST Center for Neutron Research as a post-doctoral fellow and is currently the Boeing-Roundhill Chair Professor of Chemical Engineering at the University of Washington where she has served since 2007.

Biography

Dr. Matías Rafti

Complete name: Matías Rafti (born 19.05.1979, La Plata, Bs. As., ARGENTINA)

Bachelor/Master: Chemistry/Physical Chemistry (Universidad Nacional de La Plata (UNLP) - 2003)

PhD Thesis: Heterogeneous Catalysis in UHV,: experiments and modelling (2008, Prof. Imbihl - LUH (Hannover), Prof. Vicente - UNLP)

Post Doctoral research: Prof. Migone (nanostructured carbon as advanced sorbent, Carbondale, IL, US)(2010), Prof. Matzger (MOF synthesis and applications, Ann Arbor, MI, US) (2012), Prof. Hartmann (MOFs as supports in biocatalysis, FAU-Erlangen, Germany)(2015).

Current interests: Integration of Metal Organic Frameworks with functional polymers for the creation of nanoarchitectures with applications in selective transport, sensing and energy.

Prof. Matthias Rehahn

After studying chemistry at Johannes Gutenberg University Mainz, he completed his doctorate in 1990 in the field of electroactive polymers at the Max Planck Institute for Polymer Research. This was followed by a post-doctorate and further research activities at ETH Zurich and the University of Karlsruhe (now KIT). He focused on surface and interfacial chemistry, modeling of chain dynamics, polyelectrolytes and coordination polymers. After his habilitation in 1996, he was a visiting professor at the University of Mainz from 1997 to 1998. Since 1999 he has been a full professor at the Technical University of Darmstadt. Also from 1999, he headed the German Plastics Institute (DKI) in parallel and transferred it to the Fraunhofer Institute for Structural Durability and System Reliability LBF as the “Plastics Division” in 2012. After three years as head of this division and deputy director of the LBF, he was elected Vice President for Knowledge and Technology Transfer at TU Darmstadt. In 2019, he took on the role of Scientific Director of the Helmholtz Center Hereon (formerly HZG) in Geesthacht for 5 years. The central task was to develop a new target image for Hereon. The core element of the new research strategy, which successfully spans the competencies of the entire center, was the data- and computer-assisted validation of complex technologies in complex natural environments. Back at TU Darmstadt, the development of a new research focus in the field of computational macromolecular chemistry has been underway since September 2024.

Biography

Dr. Anke G Roth

Anke Gundula Roth completed her undergraduate studies in Chemistry at Freie Universität Berlin and earned her Ph.D. in Medicinal Chemistry from Humboldt-Universität zu Berlin. Funded by the German National Academy of Sciences Leopoldina, she conducted research under the mentorship of Craig M. Crews at Yale University (CT, USA), focusing on innovative approaches to combat various cancer types over a two-and-a-half-year period before transitioning to industry. Since 2014, Anke has served as the R&D and QA Manager at Nanostone Water, a U.S.-based company dedicated to advancing technologies for clean water generation. Her research centers on the development of high-performance ceramic ultrafiltration membranes tailored for “challenging water” or “sweet spot” treatment applications, with an emphasis on minimizing energy consumption. This includes the functionalization of ceramic membranes through the application of polyelectrolyte (hybrid membranes) and the development of biofouling-resistant coatings, along with targeted process optimizations. Anke's contributions to the field have been recognized through multiple accolades, including the Fischer Nernst Award, Klaus Grohe Award, and participation in the 63rd Nobel Laureate Master Class, as well as being nominated as a Sustainable Hero and receiving the IQ Innovationspreis Mitteldeutschland. Her work is characterized by a commitment to advancing sustainable water purification technologies.

Biography

Prof. Clément Sanchez

Clément Sanchez is Emeritus Professor at the Collège de France chair of « Chemistry of Hybrid Materials » and Professor at the Institut of Advanved Studies of Strasbourg. He was Director of The “Laboratoire de Chimie de la Matière Condensée de Paris” (UMR 7574, University of Pierre and Marie Curie-Collège de France-CNRS) (1999-2013). He did a large part of his carrer at the CNRS were he was Director of Research and he was also Professor at l'Ecole Polytechnique. He received an engineer degree from l'Ecole Nationale Supérieure de Chimie de Paris in 1978 and a “thèse d'état” (PhD) in physical chemistry from the University of Paris VI in 1981. He did a post-doctoral work at the University of California, Berkeley, and is currently performing research UMR7574 in Paris and at USIAS in Strasbourg. He is specialized in the field of nanochemistry of nanostructured porous and non-porous transition metal oxide based gels and porous and non-porous hybrid organic inorganic materials shaped as monoliths, microspheres and films. He has created a new school of thought in materials chemistry and opened a new disciplinary field with both fundamental and technological impact. He has pioneered the development of functional inorganic-organic hybrid materials, synthesized via ”chimie douce” coupled with green processing methods. He was able to implement many of his fundamental concepts into technologies for hybrid materials, applied nowadays in adsorption, catalysis, protection, waste recycling and optics… He has pioneered the areas of functional hybrid-materials and sol-gel science. He created of a new ”school of tought” in materials chemistry and the reduction to practice of his fundamental concepts described in numerous patented technologies with applications in smart coatings, sensors, catalysts, membranes, waste-recycling, cosmetics, etc...

He also organized scientifically many national and international meetings associated to the field of soft-chemistry, hybrid materials and related bio-aspects. He received many national and international awards among them: the CNRS Silver Medal, the Gay-Lussac-Humboldt Award, the P. Süe Award of the French Chemical Society, the Institut Français du Petrole Award of the French Academy of Sciences, the François Sommer Award « Man and Nature », the Eni Award « Protection of the Environment », the Chemistry Blaise Pascal Medal of the European Academy of Sciences and recently the Grand Prix international de la Maison de la Chimie 2024. He is member of several Academies, among them: the French academy of sciences, The European academy of sciences, The French academy of technologies, the World academy of ceramics.

Biography

Prof. Prof. Damián Scherlis

Doctorate in Chemistry 2002, Faculty of Sciences, University of Buenos Aires.

Postdoc 2002-2005, DMSE, Massachusetts Institute of Technology Field of Research: Thermodynamics and dynamics of condensed phases using molecular simulations based on classical and quantum-mechanical approaches

Supervisor of 10 doctoral theses

75 scientific articles in J. Am. Chem. Soc., Chem. Rev., Angew. Chem., Phys. Rev. Lett., PNAS, among others (h-index 35, 4055 citations as of Sept 30, 2024)

Biography

Prof. Galo Soler-Illia

Galo Soler-Illia studied Chemistry (MSc and PhD) at Buenos Aires University (UBA) and completed a postdoc at University Pierre-et-Marie-Curie, Paris. At present, he is CONICET Superior Researcher at the Instituto de Nanosistemas, National University of San Martín (UNSAM, Buenos Aires, Argentina), which he founded and leads since 2015. He is also Full Member of academies ANCEFN, ANC and ACAL. He is Associate Professor at UBA, and Full Professor at UNSAM. He has been Invited Professor at the universities of Paris VI, Osaka Prefecture and Melbourne, and Visiting Professor at ENS-Lyon. He is a member of the Editorial Advisory Board of Chemistry of Materials, Journal of Sol-Gel Science and Technology, Hybrid Advances, and Chemical Science. He has been elected Honorary Member of Centro Argentino de Ingenieros and Fellow and Vice-President of the International Sol-Gel Society.

He has published more than 200 papers in peer-reviewed journals and books, filed five patents and made more than 100 presentations in conferences. He has supervised 23 PhD theses, more than 25 postdocs and 10 CONICET assistant researchers. He has coordinated numerous national and international projects with academic and industrial partners. He recently co-founded a technological-based company, Hybridon.

Galo has also contributed to science outreach by publishing three books and as a science specialist in radio and National TV shows. He received several national awards, including two Houssay Prizes (2006, 2009), Konex Platinum Award (2013) INNOVAR Great Prize (2016) and Bunge& Born (2022), and a Dr. h.c. from Universidad Nacional de San Luis (Argentina).

His research work is focused on the designed production of new nanosystems with intelligent architectures and custom properties using chemical methods inspired by Nature, with applications in health, environment and renewable energies.

Biography

Prof. Igal Szleifer

1984 B.Sc. Hebrew University of Jerusalem, Chemistry (cum laude)
1989 Ph.D. Hebrew University of Jerusalem (summa cum laude)
Thesis Advisor: Professor Avinoam Ben-Shaul
Thesis Topic: “Statistical Thermodynamics of Amphiphilic Aggregates”
1988-89 Visiting Scientist, Dep. of Chemistry, Cornell University (with Prof. B. Widom)
1989-91 Postdoctoral Associate, Dep. of Chemistry, Cornell University (with Prof. B. Widom)
1991-97 Assistant Professor, Department of Chemistry, Purdue University
1997-00 Associate Professor, Department of Chemistry, Purdue University
2000-07 Professor, Department of Chemistry, Purdue University
2002-07 Head Division of Physical Chemistry, Purdue University
2009-14 Associate Director, EFRC-NERC Center
2009-11 IRG-2 Leader, MRSEC Northwestern University
Since 2007 Christina Enroth-Cugell Prof. of Biomedical Engineering, Northwestern University
Since 2007 Professor, Dep. of Chemistry, Northwestern University
Since 2008 Professor, Dep. of Chemical and Biological Engineering, Northwestern University
Since 2011 Professor of Medicine, Feinberg School of Medicine, Northwestern University

Biography

Prof. Matthias Thommes

Matthias Thommes is Full Professor and Head of the Institute of Separation Science and Technology at the Department of Chemical and Biological Engineering at the Friedrich-Alexander Universität Erlangen-Nürnberg (FAU). He also served as Head of the Department for Chemical and Biological Engineering at FAU from 2021 to 2023.

Matthias obtained his Ph.D. in Physical Chemistry in 1993 at the Technical University Berlin. From 1992 to 1995 he was a project scientist at the EURECA mission of the European Space Agency (ESA). In 1996, he moved as an ESA fellow/research associate to the University of Maryland, College Park, USA. In 1998, Matthias joined Quantachrome Corp (Boynton Beach, FL, USA).and was prior to accepting the position at FAU Scientific Director at Quantachrome Corporation, Boynton Beach, USA (from 2001 to 2018). .In addition, he held Visiting Professor positions at the University of Edinburgh (UK) and the University of Lorraine (Epinal, Nancy, France) as well as prestigious leadership positions in a number of national and international boards, committees and authoritative bodies in the field of adsorption, nanoporous materials and their characterization. This includes the International Union for Pure and Applied Chemistry (IUPAC)), American Institute of Chemical Engineering (AIChE), International Zeolite Association (IZA), Facility of Adsorbent Testing and Characterization (FACT) at the National Institute of Standards (NIST, USA), International Adsorption Society (IAS), International Standard Organization (ISO).

Matthias Thommes' work involves investigating the adsorption behavior of fluids in nanoporous materials, developing methodologies for application-specific nanoporous material characterization (both in the dry and wet phase) and conducting research in gas and energy storage. Within this framework, he examines the effects of nano-confinement on the adsorption, phase and wetting behavior of subcritical and supercritical fluids in nanopores. His research forms a link between the adsorption properties of adsorbents and their characteristics with the development of nanoporous materials and their use in various processes

He has received numerous recognitions for his work, among them the induction as a Fellow of the International Adsorption Society (IAS) in 2021.and most recently by the American Institute of Chemical Engineers (AIChE), where is was distinguished for his outstanding achievements in the area of fundamentals of adsorption and porous materials characterization. during a dedicated Honorary Session on October 28th in San Diego (USA) at the 2024 AIChE Annual Meeting.

Biography

Prof. Prof. Damián Scherlis

Kristina Tschulik studied Chemistry at TU Dresden (Germany) and performed her doctoral studies on magnetic field-assisted structured electrodeposition at IFW Dresden until 2012. Afterwards, she joined the University of Oxford (UK) as a Marie Skłodowska-Curie postdoctoral Fellow, working on single nanoparticle electrochemistry and electroanalysis. In 2015, Kristina moved to Ruhr-Universität Bochum (Germany) as a Junior Professor, where she was promoted to Full Professor in 2018 and currently holds the Chair of Electrochemistry and Nanoscale Materials. Her research focusses on characterizing physical properties and intrinsic chemical (re-)activity of functional nanomaterials for renewable energy technologies by advanced electrochemical approaches including single entity electrochemistry and spectro-electrochemistry.

Amongst others, she has received the Förderpreis auf dem Gebiet der Angewandten Elektrochemie“ of the GDCh in 2012, the Early Career Grant of the International Society of Electrochemistry, section for Anayltical Electrochemistry in 2017 and was a visiting Professor at the University Paris Diderot (in 2017) and at the University of Brno (since 2023).

Kristina Tschulik received an ERC Starting grant of the European Research h Commission in 2020, is a Fellow of the Max-Planck-Society (2022), a member of the NRW “Academy of Sciences, Humanities and the Arts” (2020) and Editor of the Journal “ACS Catalysis” since 2023.

07

Statements

Prof. Markus Antonietti

I will describe quantum effect by the change in thermodynamics and kinetics. I will talk about “quantum number” pore energy storage, unusual electrocatalysis with “metallic pore hydrogen”, and how single molecules in their cavities change properties of a porous host semiconductor. In the end I will go to Japanese element theory where the void has the status of an own element.. The future of the field of course is breathtaking.

Prof. Angela Danil De Namor

Supramolecular Nanoscience and Technology for the Detection/ Removal of Pollutants from Water. Conclusions: Brief Comments about the State of the Art. Future Challenges: Water Research is one of the topics that will be in the Agenda of future research due to a number of factors among them the increase in World population and climatic changes .Therefore the need to address two main topics i) the use of naturally occurring nanomaterials as well as synthetic materials based on Supramolecular Chemistry for water sensing and technologies for water purification proceses. Particular emphasis will be placed on the implications of mercury speciation in water and consequently in food. The role of thermodynamics in these processes will be addressed.

Prof. Javier García-Martínez

The introduction of disorder into crystalline materials creates exciting opportunities in nanoconfinement engineering. Deliberate disruption of ordered structures results in novel physical properties, such as enhanced flexibility and tunable pore sizes and architectures, which can be exploited to optimise interactions between confined reactants and catalysts. The design, control and characterisation of defects within porous architectures is critical to fine-tuning these properties, as defects can enhance diffusion and surface interactions. We are working to create enzyme-like catalysts with excellent selectivity that mimic the precise confinement found in biological systems, where reactants are optimally positioned around highly accessible active sites to maximise reaction efficiency.

Prof. Stefan Guldin

Molecular self-assembly provides unique pathways to encode structural characteristics into mesoporous films. In my impulse lecture, I will present our recent efforts to extend pore dimensions, enhance pore accessibility, and minimize pore dispersity and present unique opportunities such architectures offer for enzyme immobilisation and nanopore-blockage based biosensing.

Prof. Stefan Howorka

Nanofluidic transport across confined space is relevant for nanopore-based DNA sequencing and single-molecule sensing as well as for filtration with multipore membranes for food processing and purification of water and medicine. The Impulse presentation will delineate how nanofluidics in these different pore systems can be better understood to create synergistic crosstalk and develop advanced membranes for existing but also new applications.

Prof. Laurent Joly

Molecular simulations, by their very nature, are approximations and will never fully capture the complexity of reality. However, this inherent limitation may not be a drawback. Simulations can still serve as powerful tools, offering insights that inspire and refine theoretical models. Rather than aiming for absolute accuracy, they can guide our understanding of complex phenomena, helping us develop theories that reveal the underlying principles governing the physical world. This work station will explore how the value of simulations lies not in perfect representation, but in their ability to inform and drive theoretical innovation.

Statements

Dr. Christian Kuttner

Disruption versus Consolidation? An Editor's Perspective on Scientific Progress

In the field of nanoconfined chemistry, researchers are often torn between pushing the boundaries with disruptive ideas or consolidating existing knowledge for steady, incremental progress. My talk will explore how we, in my case from the perspective of a edior, navigate this tension when evaluating scientific contributions. Drawing on recent examples from the literature, particularly in the areas of nanoporous materials and nanoconfinement, I will illustrate how we assess research for its potential to drive the field forward whether through groundbreaking discoveries or the refinement of established theories.

This talk aims to transition into a dialogue with the audience, discussing how authors, reviewers, and editors can collaborate to move the field forward more efficiently. By sharing experiences and insights from the editorial process, I hope to open a conversation on how we can collectively shape the future of nanoconfined chemistry, making the most of both disruptive innovations and essential consolidations. Audience interaction will be encouraged throughout, fostering a dynamic exchange on the challenges and opportunities that lie ahead in advancing this vital field.

Prof. Stefan Lamotte

Chromatography and especially liquid chromatography is one of the most important use cases for silica. It is the most important analytical technique for the quality control in pharmaceutical industry as well as for food, feed, consumer care and agricultural industry. Silica for these applications is surface modified and packed into metal tubes called “separation columns”. Liquids are pumped with high pressure (up to 150 MPa) through theses columns and mixtures are injected and separated on these columns. A reproducible manufacturing of these columns is the key element for a validation of a liquid chromatographic method in industry. Improvements in performance are done over the years. However, still a lot of trial and error and empirical efforts are done to manufacture the silica materials in the required physicochemical specifications. Challenges are to design materials with narrow particle size distribution, pore size and pore volume as well as specific surface area.

Prof. Serge Lemay

Confinement can greatly influence electrocatalytic processes, as the high surface-to-volume ratio inherent to nanochannels means that surface effects take a much more prominent role in the transport of both solvent and ions. Phenomena that can become dominant include for example reversible adsorption, streaming currents and surface conduction. Currents need not necessarily be driven by an electric field, but can also be caused by gradients in pressure or concentration. The converse is also true: ion transport near a charged surface leads to convection in the form of electroosmotic flows. Fluid and charge transport thus become intrinsically linked under confinement. Disentangling these effects in nanostructured, disordered materials such as are employed in realistic applications represents a formidable challenge.

Statements

Prof. Bettina Lotsch

Materials are vital ingredients to solve societal challenges and drive innovation and new technologies. Historically, porous materials have played an important role in large-scale processes including the production, transformation and valorization of platform chemicals (e.g., zeolites), but also in the production of specialty chemicals, biomedical applications, and sensing.

To produce the next generation of porous materials and leverage confinement effects for specific applications, a number of materials challenges will have to be addressed, which range from the discovery of new porous materials with well defined, robust and functional pore systems and elucidation of their structure-property-function relationships to the synthesis of hierarchically structured materials and the development of scalable production processes.

This can only be achieved in a tight feedback loop with materials characterization and modelling and is contingent on our ability to exquisitely control material design and function.

The following challenges come to mind:

-Leverage the complexity of the materials space to synthesize materials with precisely defined pore shapes, sizes and pore topologies, which at the same time are robust and scalable. Examples are metal- and covalent organic frameworks (MOFs, COFs), but also porous polymers and hydrogen-bonded frameworks.

-Develop hierarchically structured pore systems with interconnected pores fulfilling multiple functions, for example distinct reaction and transport pores.

-Use data-driven and automated synthesis procedures to develop both reproducible and scalable synthesis protocols.

-Establish protocols for discriminating between surface and pore-reactivity and for exploring confinement effects operating in different pore size regimes to ultimately tailor pore properties (size, shape, functionalization) to specific tasks and processes.

Prof. Shlomo Magdassi

Impulse presentation: Material fabrication today and tomorrow work station I: New fabrication technologies such as additive manufacturing

• New fabrication technologies enable confinement in sub-micron to large-scale structures

• Combining materials-based structuring within printed objects enables hierarchical confinements

• New applications emerge by combining new materials with advanced printing technologies, such as structural glasses, ceramics, catalysts, hybrid aerogels, and stretchable foams, for example, in optical devices, catalysts, sensors and insulators.

• Multi-material printing enables combining structuring and chemical confinement.

Statements

Prof. Kazuki Nakanishi

Discussed will be the importance and challenges of integrating nanoconfined structure into larger scale assemblies in a controlled manner. The assembling process is desirably simple, quick and low-cost, by utilizing spontaneous structure formation phenomenon such as phase separation. Examples of spinodal decomposition in various sol-gel systems will be explained for further discussion.

Nanoconfined substances needs controlled contact with external substances. The “vessel” of confining functional substances should be architected into larger scale structure. Spontaneous structure formation process can replace highly sophisticated energy-intensive fabrication process.

Prof. Sebastian Polarz

Catalysis benefits from multiple confinement effects. Unlike biocatalysis, the existing synthetic systems hardly exhibit adaptive characteristics. This means that nanoreactors and the associated confinement conditions react dynamically to the ongoing chemical processes.I propose fluctuating confinements linked to chemical evolution. This way, dynamic nanoreactors could scan the entire parameter space and enrich in a structure which is self-optimized for a particular chemical reaction.

Prof. Lilo Pozzo

"Integrated human creativity, automation and data science for accelerated materials design and discovery"

The integration of human knowledge and creativity with accessible laboratory automation and modern methods in data analysis and artificial intelligence (AI), has significant potential to accelerate materials optimization in multidimensional chemical design spaces. This impulse talk will demonstrate the use of key tools that can be adopted broadly to advance the science of synthesis and assembly of nanostructured and nanoporous materials. We demonstrate the integration of synthesis and analysis (e.g. spectroscopic and scattering) with modern algorithms for autonomous decision making and adaptive design of experiments.

Statements

Dr. Matías Rafti

Designing Confinement Features with Nanobuilding Blocks: A Data-Driven Approach to Synthesis

A clear example of the advantages and limitations of data-driven research can be traced back to the last decades of the twentieth century. The surface science and solid-state physics community developed a range of analytical tools specifically designed to scrutinize interactions occurring at the single-atom level through the use of ultra-high vacuum (UHV) conditions. One of the main goals was to achieve a deep understanding of heterogeneously catalyzed reactions by reducing the complexity of industrial-scale processes using custom single-crystalline catalysts and low pressures (i.e., low coverages). This approach proved successful in generating fundamental knowledge regarding reaction mechanisms and detailed interactions between adsorbates and various catalysts.

Moreover, a virtuous feedback loop between theory, simulations, and experiments was established, leading to the application of methods such as density functional theory (DFT) calculations, numerical simulations, and even the creation of databases containing information on correlations between chemical features and functional properties. The greatest challenges the field faced - challenges that are still only partially addressed today - were the need to fill the so-called material and pressure gaps. The behavior of real-life catalysts differs from idealized systems due to the effects of high operating pressures and, more notably, the complexity of real-life catalysts compared to perfectly ordered single-crystal structures. Unfortunately, while many of the approximations employed for modeling idealized catalysts are generally useful, they are often inadequate for conditions relevant to anticipated applications.

In a similar vein, a number of predictive tools based on ab initio calculations and artificial intelligence (AI)-assisted algorithms have become available in the last decade, and they have been employed to accelerate research related to porous nanomaterials (PNs). Notable examples of the numerous possibilities offered by PNs include their incorporation into nanoarchitectures that confer selectivity for separation and sensing technologies in gas or liquid phases. A particularly interesting case involves the integration of microporous polymers and metal-organic frameworks (MOFs) into solid-state nanopores (SSNs), resulting in nanoarchitectures with overlapping porosities; that is, it combines the inherent transport properties of SSNs with additional modulation provided by the embedded MOF phase.

Much like the previously discussed "material gap" problem in surface science, the ab initio tools employed for describing transport properties in MOF-filled SSNs assume an ideally completely filled nanopore, i.e., a single crystal of MOF. This approach is tempting as it allows for significant generalization regarding the energies required for hydrated ions forced to fit through perfectly aligned apertures into pores that can then act as size-selective media. Recent experiments conducted on MOF@SSNs suggest that such idealization cannot capture the complexity of the observed behavior, as the combination of transport dynamics through a perfectly ordered microporous continuous phase must be complemented by the presence of mesoporous channels that are naturally (and inevitably) formed during MOF synthesis.

Although the significance of this so-called “constructional” mesoporosity has been suggested in the literature, it has only recently been linked to the observed transport mechanisms. This "real-life" effect bears a striking resemblance to the previously discussed examples and highlights a common challenge that warrants specific discussion: the limitations and advantages of tackling complex problems using first-principles calculation methods.

Statements

Prof. Matthias Rehahn

Work Station II: ML/AI/Digital Twins: Hype or Added Value?

Structures and architectures on the nanoscale have long exerted a great fascination in the natural and technical sciences. Numerous counterparts from nature as well as expectations with regard to their potential uses have repeatedly given rise to major research activities in the past. A few years later, however, it had to be stated that only a small part of the hopes could be fulfilled, while many others failed due to initially unnoticed hurdles. In favorable cases, unexpected innovation potentials were recognized in the course of research. However, these could then only be pursued with a delay or with fewer resources.

Looking back at (i) the progress of knowledge, (ii) the impact of innovation and (iii) the use of resources, especially in the nano-hypes, it must be said that many wrong turns could have been avoided and opportunities should have been seized much earlier. However, research planning should have been much more interdisciplinary and open in the early stages - something that has been virtually impossible to implement to date. Recently, however, a way has opened up for the first time to massively increase the efficiency of research, particularly in such highly innovative and high-risk fields as nanoconfinements, and to pave the way for their implementation in successful innovations:

Using large data sets, mechanistic understanding, AI and ML tools, so-called “digital twins” of the desired nanostructures will be developed via modeling and simulations. These digital object twins are in permanent feedback loops with their physical counterparts and are continuously improved in terms of the sharpness of the image of the real object. Subsequently, these digital object twins will be gradually embedded in increasingly complex system environments. This starts, for example, with the integration of the initially isolated nanostructures into larger arrays and extends to the consideration of the nanoconfinement system in the system environment - also developed as a digital twin - of the respective practical application, including all the disturbance variables to be expected there.

Such a complex “overall system twin” is continuously refined by mirroring selected physical counterparts, and ideally will show whether a path is worthwhile and which plan adjustments may be necessary even before extensive laboratory and practical research. In the future, this overall system twin will not only identify the less promising research approaches at an early stage, but will even make it possible to evaluate ageing processes, predict desired and undesired feedback on the system environment or validate hypothetical scenarios without any preliminary experimental work and thus explore potentials for which no resources would be available on the basis of physical experiments.

The latter new possibilities are particularly relevant in light of the claim that nanoconfinement research will address “major global challenges”. Not only would fields such as water, energy, medicine/medical technology or material synthesis gain immense additional momentum, but we could also expect much more central and versatile contributions to sustainable and resilient solutions to the “global grand challenges” such as climate change, species extinction, demographic changes, global pollution and resource security.

In summary, the exorbitant benefits of this novel approach to scientific and technical research questions with the help of digital twins would be (i) the early identification of really worthwhile priorities, (ii) the avoidance of scientific dead ends and (iii) the exploitation of additional potential uses for which there would be no opportunities in the context of classical research, and thus (iv) the massive increase in the focus and efficiency of such research. It would also be possible to make a well-founded argument in this specific case as to why (v) nanoconfinements are a unique key “component” and why (vi) the development of a special community for this is recommended. Not to be forgotten would also be (vii) the significantly earlier identification of implications that are required, for example, for approvals or social discourse - often unrecognized show stoppers, especially in fields of the highest level of innovation. Finally, such an approach in the field of nanoconfinements - if it starts promptly - would benefit massively from parallel developments in the fields of climate and implant research, for example.

Statements

Dr. Anke G Roth

REMOVAL OF PHARMACEUTICALS FROM AQUEOUS SOLUTIONS USING HYBRID CERAMIC MEMBRANES

The provision of clean, pollutant-free drinking water is increasingly challenged by anthropogenic contaminants, notably pharmaceutical residues (e.g., diclofenac, bezafibrate, carbamazepine, various hormones, and contrast media) and agricultural antibiotics. This issue is further exacerbated by the heightened consumption of medications in aging populations within industrialized nations and the proliferation of micro- and nanoparticles, which complicate separation processes and necessitate advanced technological solutions. To address the stringent demands for water quality, innovative approaches to water treatment are imperative, thereby necessitating sustainable water management strategies on a global scale.

This study investigates the applicability of novel hybrid membranes for the effective separation of micropollutants from aqueous solutions. These membranes integrate the technological benefits of ceramic filtration elements with polyelectrolyte films, specifically engineered for the removal of pharmaceutical contaminants. The ultrafiltration alumina ceramic membranes were coated with nanoscale polyelectrolyte films via layer-by-layer assembly. This method involves the sequential application of thin polyelectrolyte chains onto the ceramic substrate, resulting in the formation of a nanoporous network. This engineered structure enhances the retention capabilities for small molecules, including pharmaceuticals and microplastics, which are typically inadequately removed by conventional ultrafiltration techniques.

Comprehensive comparisons were conducted between the original ultrafiltration ceramic membranes and the newly developed hybrid membranes, focusing on key properties such as permeability, pore size distribution, and zeta potential. The electrostatic interactions and repulsion of the membranes against oppositely charged contaminants were characterized using streaming potential techniques. Filtration behavior emerged as a critical parameter in the overall membrane characterization, with retention studies indicating significant efficacy in the removal of prevalent pharmaceuticals, including diclofenac, ibuprofen, and sulfamethoxazole.

The findings of this study contribute a novel perspective to the discourse on nanoscale contaminant removal from aqueous systems and underscore the potential for employing advanced membrane technologies to enhance the efficacy of water treatment processes aimed at mitigating pharmaceutical pollution in drinking water supplies.

Statements

Prof. Clément Sanchez

Tailor-Made Materials and Methodologies for Advancing the Understanding of Confinement Effects

Confinement effects are central to the behavior and properties of a wide range of materials and systems, particularly in porous materials, hierarchical porous structures, nano-objects, and biological channels. These effects arise when the spatial constraints imposed by the surrounding structure lead to unique physical and chemical phenomena, significantly altering material properties and enabling new functionalities. Confinement effects depend on the relative sizes of the host and the guest. For humans, these effects become significant when the host size is less than about one meter. However, for molecules and macromolecules, such effects are noticeable at sizes below 10 nanometers."

Key Areas Where Confinement Effects Play a Critical Role:

• Catalysis: In confined spaces, catalytic reactions often exhibit altered pathways and enhanced selectivity. Confinement can improve reaction efficiency by controlling the local environment around the catalyst.

• Separation Processes: The performance of materials in separation technologies, such as filtration, adsorption, and gas separation, is heavily influenced by confinement, which impacts permeability and selectivity.

• Fluid Dynamics: At the nanoscale, the behavior of fluids in confined geometries deviates from classical models. This affects transport properties, viscosity, and flow dynamics, making it important for applications in microfluidics and nanofluidics.

• Nucleation and Growth of Nano-Objects: Confinement influences the nucleation and growth of nanomaterials, dictating their size, shape, and distribution, which in turn impacts their properties and potential applications.

• Surface Chemistry of Colloids and Nanoparticles: Confinement can alter the surface interactions of colloidal particles and nanoparticles, which is critical for applications such as drug delivery, biosensors, and materials design.

IUPAC Classification of Porous Solids Based on Pore Size:

Porous materials are classified into three categories based on their pore size, each with distinct characteristics and applications:

• Microporous Materials: Pores with diameters smaller than 20 Å (angstroms)

• Mesoporous Materials: Pores between 20 Å and 500 Å

• Macroporous Materials: Pores larger than 500 Å

The specific surface area of these materials, typically measured by nitrogen adsorption (N_2), can range from as low as 5 m^2/g to over 8000 m^2/g, depending on the material's structure and porosity. This variability is key to the vast range of applications these materials can serve.

Statements

Applications of Porous and Nanomaterials:

Porous and nanomaterials are integral to a diverse array of industries due to their unique properties, among them:

• Energy Storage and Conversion: The high surface area and tunable pore structures of porous materials enhance the performance of batteries, supercapacitors, and fuel cells, driving advancements in energy storage technologies.

• Environmental Remediation: Porous materials are employed for the adsorption and removal of pollutants from water and air, membranes, making them vital in environmental cleanup and sustainable technologies.

• Biomedical Applications: Their ability to selectively interact with molecules and cells makes porous and nanomaterials ideal for drug delivery systems, biosensing, and tissue engineering.

Key Parameters for Characterizing Porous Materials:

1. Pore Size Distribution: The distribution of pore sizes is critical for optimizing material properties such as adsorption capacity, permeability, and catalytic efficiency.

2. Network Connectivity: The degree to which the pores are interconnected within a material affects transport properties (e.g., diffusion and flow) and mechanical strength.

3. Wall Composition and Functionalization: The chemical composition and functionalization of the walls of porous materials (using organic or inorganic groups) can significantly alter their surface reactivity and stability. This ability to modify the surface chemistry is essential for tailoring materials to specific applications.

For instance, Zirconium cyclosilicate (ZS-9) is a material used in the treatment of hyperkalemia, a medical condition characterized by elevated potassium (K^+) levels in the blood. The porous structure of ZS-9 allows it to selectively adsorb potassium ions, lowering their concentration in the blood and restoring a normal electrolyte balance.

Addressing the Challenges in Understanding Confinement Effects:

To improve our understanding and exploitation of confinement effects, several key advancements are needed:

• Development of Model Systems with Tunable Complexity: The creation of materials with precisely engineered structures that exhibit specific confinement effects will allow for controlled studies and a deeper understanding of these phenomena.

• Enhanced Characterization Techniques: Advanced characterization tools, such as high-resolution imaging and spectroscopy, are crucial for accurately determining pore structures, surface chemistry, and dynamic behaviors at the nanoscale.

• Refinement of Theoretical Models: Current models need to be adapted to account for the complexities of real-world materials and systems. This includes incorporating multi-scale, dynamic effects and developing predictive models that closely align with experimental data. Both thermodynamic and kinetic descriptors are important to use.

Statements

Prof. Damián Scherlis

► Nanoconfinement is an invitation to molecular simulations

The scientific and technological drive toward smaller structures demands instruments capable of providing high resolution in space and time. This is precisely the realm of molecular simulation methods, conceived to interrogate matter at the nanoscale. State of the art approaches have attained such a level of accuracy as to become the natural instrument to interpret experiments, providing information not accessible through any other technique. In particular, nanoscale confinement alters practically every physical chemical property of water that has been experimentally probed, from transition temperatures and heat capacity to dielectric constant and chemical reactivity. Simulations have been an essential piece in this exploration, by providing a microscopic insight complementing experiments. The present knowledge and understanding of the physical chemistry of nanoconfined water would be unconceivable without the power of molecular modelling.

► Where can modeling contribute? Opportunities for theoretical/experimental feedback

It is possible to highlight four clear dimensions where theoretical approaches can provide insight in confined systems: (i) spectroscopy, (ii) thermodynamics, (iii) transport, (iv) reactivity. The former and the latter typically require first-principles or QM-MM approaches. The other two involve larger length and time-scales, and are usually tackled with atomistic or coarse grained potentials, deployed through molecular dynamics or Monte Carlo schemes. Continuum or multiscale models can be important specially for transport. Examples of the kind of infornation attainable in each case follow (this list is not exhaustive) :

(i) Spectroscopy: IR, UV-vis, Raman, Fluorescence, NMR, Circular dichroism, among others.

(ii) Thermodynamics: phase transitions, solubility, dielectric constant, adsorption isotherms, phase transitions

(iii) Transport: diffusion coefficients, residence times, transport mechanisms

(iv) Reactivity: equilibrium, reaction energies, free energies and entropies, mechanisms, rate constants.

► What is the current state of the art, what lies ahead? More questions than answers

At the present stage, modeling is a clear complement to experiments. It is extremely useful for interpretation and understanding. However, is it predictive? Can it be applied as a standalone tool, bearing the same status as an experimental technique. I think yes it can, but in a limited and specific number of cases. Confined chemical systems are complex and large from the perspective of molecular simulations, and at the moment they may be erratic when it comes to quantitative data. But they can also be very reliable to anticipate relative trends, for instance: how a barrier or a signal is affected with a change in some condition. Or among different possible chemical designs, which one is most likely to achieve a particular property?

Is modeling going to become predictive in a quantitative sense, and in a near future? Much of the expectation relies on machine learning potentials, including reactive force fields, as well as linear scaling and more efficient quantum chemistry/electronic structure methods. In parallel, high throughput/data-mining tools proliferate, however, are they being used? Will they be? We are at a stage where traditional meticulous scientific procedures coexist with automated processing tools and massive data analysis. The question is whether this is a transient stage that will evolve into something else, or if the trend will consolidate and this coexistence will remain with us for long.

Statements

Prof. Igal Szleifer

Past and ongoing efforts focused on modeling the structure and transport properties of chemically modified nanopores and nanochannels using molecular theories. Previously, we modeled the structure of synthetic pH-responsive polyelectrolytes functionalized nanopores and biological nanopores (nuclear core complexes). We investigated properties such as cargo (nanoparticle) translocation and ion conduction.

For example, Qin et al., in ACS Nano 2022, and Huang et al., JACS, 2017, demonstrated theoretically the possibility of using pH-responsive polyelectrolytes functionalized nanopores for current rectification and pH-controlled gating. This follows Tagliazucchi et al., JACS 2011, seminal predictions and experimental verification of pH-controlled conduction of nanopores.

Very recently, Gonzalez Solveyra et al., ACS Nano, 2024, showed that the adsorption and release of proteins (GFP, lysozyme, RNase, and beta-lactoglobulin) by a pH-responsive polyelectrolyte functionalized nanopore (NP) depends on the pH, salt concentration, and acid-base equilibrium of protein's amino acid and polyelectrolyte layer, the amino acid composition of the proteins as well as the degree of polymerization, density of the polyelectrolytes inside the NP. Depending on the type of protein, adsorption and release occur at different reservoir pHs and salt concentrations.

Reason: charge regulation involving the acid-base equilibrium reactions of the functionalized polyelectrolytes inside the NP and the amino acid groups of protein are coupled and influence the ensuing electrostatic interactions. The interplay between acid-base reactions of the polyelectrolytes and amino acids of the proteins affects the charge and electrostatic interactions and, thereby adsorption, release, and translocation of proteins. External salt concentration and pH modulate these interactions. The rectification and pH-controlled gating and ion conduction arise from a similar coupling of chemical acid-base reaction and structural organization.

Potential applications based on these predictions and phenomena involve protein sensors and detection devices. Separation of proteins and filtration of protein mixtures for purification. Other applications can be delivery and controlled release devices and bioreactors.

The rectification, gating, and pH-controlled conduction properties of functionalized nanopores can be utilized to build ionic circuits for example for autonomous sensing.

The interplay between chemical interactions and physical interactions determines the structure and transport properties of chemically modified nanopores. Unraveling this interplay requires both theoretical modeling and experiments to determine the (most) relevant control and nanopore design parameters.

Relevant nanopore design parameters involve

• Geometry: cone, cylindrical, 'oscillating' pore,…

• Functionalization: weak –polyelectrolytes, surfactants, surface acid/base moieties, …

• Substrate: dielectric, metal, polymer membrane, mineral, …

• External Conditions: pH, salt concentration, Steady-state versus equilibrium, Concentration gradient in salt of pH, Applied electrostatic potential difference.Osmotic flow

Statements

Prof. Matthias Thommes

Nanoporous materials (pore width < 100 nm) such as activated carbons, zeolites, metal organic framework materials, ordered and hierarchically structured meso-macroporous oxides have been the subject of extensive research targeted towards energy and environmental applications because of to their unique textural properties such as increased surface area and the ability to customize the pore size and pore size distribution. In addition, unique nano-confinement effects, such as for instance enhancements in the adsorption capacity, reaction kinetics, ion selectivity and gas solubility can be observed within narrow nanopores. Moreover, confinement induces shifts in the phase diagram of pore fluids and alters their thermophysical properties.

Whereas in narrow micropores (pore width < 2 nm) the sorption behavior is dominated entirely by the interactions between fluid molecules and the pore wall, sorption in mesopores (pore width 2—50 nm) depends also on the attractive interactions between fluid molecules, which may lead to shifted vapour-liquid, vapour-solid and liquid-solid transition. A wealth of novel phenomena concerning the adsorption, phase- and wetting behavior and the critical point of the fluid in the pore has been predicted and observed. However, in order to utilize effects of nano-confinement in many areas of applications (e.g, separation, catalysis, gas-energy storage) a detailed understanding of the interplay between effective fluid-fluid and fluid-(pore) wall interactions on the one hand and the effects of confined pore space and poregeometry/pore network on the other hand is required.

Prof. Kristina Tschulik

Main research interest: How can we utilize confinement induced property changes to control reactivity and selectivity in in (electro)catalysis?

Key question I’d propose addressing in a consortium:

Can confined systems be designed such that confining “walls” alter reactant properties significantly, while maintaining sufficiently fast mass transport to achieve high/ industrially relevant reaction rates.

Questions for smaller sub-groups:

-Do suitable descriptors exist that allow to describe and compare different aspects of confinement based on their effect on specific properties in a general way?

-To which extend can we predict confinement induces property changes to date?

-Which key developments are required to enable prediction of confinement effect reactivity changes for (electro)catalysis?

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Notes

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Thank you to all participants and speakers for making this workshop successful, and to everyone in the organisatory team for your support in arranging this workshop.

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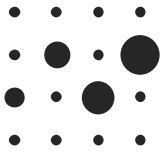

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