

3rdAnnual PANACEA the fundamentals of solid-state NMR.



user from University of Cambridge, UK.



& solid-state DNP-NMR in focus.

studied by solid-state NMR.



community.

Engaged students at the PANACEA Summer school on solid-state NMR



The 2024 PANACEA summer school immersed 68 participants in the fundamental theories and applications of solid-state NMR spectroscopy to essential and complex challenges in material science. The format and the setting, the course was held on the island of San Servolo in Italy, encouraged everyone to engage in group and round table discussions and stimulated interactions and discussions among the students and the teachers .

The program focused on the fundamentals of solid-state NMR spectroscopy for chemists and featured lectures on quantum mechanics, NMR Hamiltonians, DFT calculations and practical sessions covering pulse programming and MAS NMR. A broad range of topics was addressed, including Hamiltonians in solid-state NMR, magic angle spinning, principles of recoupling and decoupling under spinning conditions, relaxation in the solid state and DFT calculations.



A huge thank you to our esteemed guest speakers: professors Mathies, Levitt, Vosegaard, Hope, Grandinetti, Mueller, Copéret, Lewandowski, Polenova and Grey, and Drs. Perrone and Althoff from Bruker.

PANACEA key numbers

- 1650 access days 27 spectrometers
 - > 200 chemistry-related projects
- 4 user meetings
- 4 hands-on trainings
- 1 NMR summer School
- 3 industry-targeted workshops
- 32 taster days for industrials
- 8 summer fellowships for students

PANACEA 3rd Annual users meeting - a uniting experience



The PANACEA Annual users meeting, a European forum for high-level discussions between academic and industrial users and consortium partners on the latest developments in solid-state NMR spectroscopy and their applications in contemporary chemistry and materials research, was held in Aveiro, Portugal in September 2024.

The collaborative spirit was evident throughout the event, as participants engaged in discussions sparking new ideas and collaborations for the next steps of the project. We wish to thank all participants, speakers, and organizers who contributed to the success of the PANACEA Annual users meeting!

The program centered around solid-state NMR for energy materials and sustainability, for inorganic and hybrid materials, instrumentation, pharmaceurical research and methods development and was very well received.

The presentations provided a comprehensive overview of the broad applications of solid-state NMR and the attendees were treated to insights that promised to shape the future of research endeavors in the PANACEA community. In addition, a round table discussion was organized to foster sustainability models for European research infrastures, followed by a user forum.

The consortium is looking forward to welcoming you again next year to the 4th PANACEA users meeting in Gotheburg, Sweden!

PANACEA user profile

The CRMN-Lyon facility has welcomed Kathryn Gerl from the University of Cambridge, UK. We took the opportunity to get her perspective on being a PANCEA user.

Q1: Where are you from and what is your field of research?

I am currently a second-year PhD student in professor Melinda Duer's research group within the Department of Chemistry at the University of Cambridge. My research investigates how mechanical strain affects the structure and orientation of extracellular matrix proteins, such as collagen. I am particularly interested in how these mechanical changes impact osteosarcoma cell behavior, including adhesion and migration.

Q2: Could you tell us a bit more about your scientific academic journey?

I obtained my honors bachelor's degree in chemistry with an option in pre-med from Oregon State University in Corvallis, Oregon. As part of the Honors program, I completed my thesis focused on investigating novel natural products and their effects on proteostasis in various types of human breast cancer. My passion has always been in both biology and chemistry, particularly in research that bridges these two disciplines. Therefore, I am interested in using solid-state NMR to investigate the structure and dynamics of complex biological systems.

Q3: How did you hear of PANACEA?

We began a collaborative project with Dr. Danielle Laurencin from the Institute Charles Gerhardt to explore the use of ¹⁷O NMR to investigate the dynamics of biological systems. Danielle suggested that we join the PANACEA project as it offers the advanced instrumentation and expertise required to perform the challenging and complex ¹⁷O NMR experiments on our biological samples.

Q4: What was the purpose of your visit?

Our goal was to use ¹⁷O NMR to study hydrogen bonding, a critical interaction that supports the secondary structure of many proteins, including collagen. Danielle's group in Montpellier successfully synthesized ¹⁷O-labelled L-proline, which we used to isotopically enrich cell-derived collagen. This provided an exciting opportunity to explore the dynamics of hydrogen bonding within biological systems.



••• We had a wonderful experience in Lyon! The team at the NMR Center gave us a warm welcome and ensured our experience was smooth and effortless. The engineers and facility staff provided outstanding expertise, patience and support, especially when challenges arose due to the complexity of our biological samples.

Thanks to their help, we were able to collect novel spectra and detect ¹⁷O signals in collagen for the first time. This paves the way for exciting future research using ¹⁷O NMR to investigate hydrogen bonding within collagen across various biological systems and conditions.

DNP enhanced solid-state NMR and Paramagnetic NMR upcoming PANACEA workshop



A hands-on DNP enhanced solid-state NMR and paramagnetic NMR workshop will be held at the CRMN in Lyon from May 19 - 23, 2025 as part of our PANACEA training opportunities. Open to a maximum of 30 participants, the workshop is focused on the theoretical and practical aspects of both techniques. The format provides an excellent opening for early-stage researchers to discuss with international experts.

The workshop is open to PhD students, post-docs and industrial scientists who are already familiar with solid-state NMR techniques and intend to expand their knowledge and skills in terms of more advanced methodology or specific applications involving quadrupolar nuclei.

Participation is free of charge and includes meals during the workshop, but attendants must pay for their own travel and accommodation expenses.

Application will open closer to the date of the workshop at www.panacea-nmr.eu

Publication highlight: Ga-based PDH catalysts

An exciting new publication has emerged from within the PANACEA consortium.

As described by the authors, Ga-based propane dehydrogenation (PDH) catalysts are explored in industry as an alternative to PtSn and CrO_x -based catalysts. At present, there is only limited understanding of the structural dynamics of surface sites in Ga-based PDH catalysts.



The authors have used a comprehensive set of NMR applications and other methods: ⁷¹Ga MAS NMR, Ga K-edge XANES and EXAFS, Py ¹⁵N DNP SENS, Py-FTIR, CO-FTIR and H₂ dissociation followed by FTIR. In short, the authors have employed atomic layer deposition to engineer a sub-monolayer of Ga species on dehydroxylated silica, which serves as a model PDH catalyst. The results show evidence for a thermally-induced conversion of silica-supported sub-nanometer $Ga_xO_y(OH)_z$ clusters consisting of ^[4]Ga_(Ga) and ^[6]Ga_(Ga) sites, to a silica surface dominated by isolated ^[4]Ga_(4si) sites, i.e., surface gallosilicate.

MAS-NMR experiments on ⁷¹Ga were performed using 850 MHz and 1 GHz Bruker NEO spectrometers. Materials were packed into 1.3 mm diameter zirconia rotors inside an argon-filled glovebox. The rotors were spun under pure nitrogen, with experimental times typically between 15 - 48 h. In general, the nuclei of ⁷¹Ga exhibit large quadrupolar interactions, leading to line broadening and a reduction of sensitivity, requiring in turn the use of fast MAS and high fields.

Dynamic nuclear polarization surface enhanced ¹⁵N NMR spectroscopy (¹⁵N DNP SENS) measurements were performed at 8 kHz MAS spinning rate on a 600 MHz Bruker instrument equipped with a DNP triple-resonance probe coupled to a 395 GHz gyrotron microwave source to drive the DNP cross-effect.

Reference: Zixuan Chen, Alexander I. Serykh, Agnieszka Kierzkowska, David Gajan, Scott R. Docherty, Alexander V. Yakimov, Paula M. Abdala, Christophe Copéret, Pierre Florian, Alexey Fedorov and Christoph R. Müller. Reversible transformation of sub-nanometer Ga-based clusters to isolated ^[4]Ga₍₄₆₎ sites creates active centers for propane dehydrogenation, *Catal. Sci. Technol.*, 2024, **14**, 379–390.

Outreach at the European Material Research Society spring meeting

Two members of the PANACEA team, Pierre Florian and Mariana Sardo, attended the Spring Meeting of the European Materials Research Society (E-MRS) in Strasbourg in May, organized in collaboration with the Foundation Jean-Marie Lehn.

This visit proved to be a compelling community-building occasion where PANACEA was introduced to a broader array of stakeholders, encouraging new connections and potential collaborations with future users.

The conference centered around recent advances in the field of materials science in an international setting, covering decarbonized energy and sustainability, materials for human well-being, 2D materials and surfaces, materials sciences for cultural heritage and electronics, magnetics and photonics.

The meeting provided an exceptional platform to present and disseminate the diversity of opportunities offered by the PANACEA project. Florian and Sardo were on hand to address inquiries related to transnational access activities, community-building initiatives, and the various opportunities PANACEA extends to both academic and industrial profiles.

