AstroChemical Newsletter #119

December 2025

You can access the full abstracts by clicking the paper titles. Submit your abstracts before the 25th of each month for inclusion in the following newsletter.

Abstracts

Nitrogen-bearing species on trans-Neptunian objects revealed by JWST/DiSCo-TNOs

S. Cryan, R. Brunetto, A. Guilbert-Lepoutre, N. Pinilla-Alonso, E. Hénault, B.J. Holler, Y.J. Pendleton, D.P. Cruikshank, Dr. John A Stansberry, J.P. Emery, L.T. Mcclure, J. Licandro, V. Lorenzi , T.G. Mueller, N. Peixinho, B. Harvison, C.A. Schambeau, M. Bannister, A.C. de Souza-Feliciano, M. De Prá

CN-bearing species are valuable tracers of nitrogen chemistry in the Solar System. Ranging from volatile compounds like HCN and CH3CN in cometary comae to refractory CN-bearing organics in some micrometeorites and interplanetary dust particles, these species originate in, or are derived from, molecular precursors in the interstellar medium (ISM). The icy surfaces of medium-sized trans-Neptunian objects (TNOs) represent an intermediate stage in the chemical evolution and incorporation of N-bearing molecules from the ISM into the Solar System. Herein, we investigate the nature, distribution, and origin of CN-bearing species on several TNOs and one centaur observed within the James Webb Space Telescope DiSCo-TNOs program. We find a spectral feature at 4.62 um consistent in band position and width as OCN- observed in the ISM and the laboratory. This feature is most pronounced on TNOs in the Cliff2 group (Cliff2-TNOs, a compositional subgroup characterized by low ice content that include the Cold Classical TNOs, suggesting they formed farthest from the Sun) and might be tracing an original chemical inventory in the protoplanetary disk. Cliff2-TNOs are also the best candidates for studying the contribution of refractory CN-containing organics to a broad 4.5 um spectral feature. Finally, a close spectral resemblance between Cliff2-TNOs and the centaur in our analysis, which exhibits both the 4.62 and 4.5 um bands, provides a plausible dynamical channel that can enrich the inner Solar System with N-bearing species. Our work advances the understanding of N-bearing species in the Solar System and their evolutionary history beginning in the ISM.

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Formation of Unsaturated Carbon Chains through Carbon Chemisorption on Solid CO

Masashi Tsuge, Germán Molpeceres, Ryota Ichimura, Hideko Nomura, Kenji Furuya, and Naoki Watanabe

The interaction of carbon atoms with solid carbon monoxide (CO) is a fundamental process in astrochemistry, influencing the formation of complex organic molecules in interstellar environments. This study investigates the adsorption and reaction mechanisms of carbon atoms on solid CO under cryogenic conditions, employing a combination of experimental techniques, including the combination of photostimulated desorption and resonance-enhanced multiphoton ionization and infrared spectroscopy, alongside quantum chemical calculations. The results reveal the formation of oxygenated carbon chains, such as CCO, C3O2, and C5O2, as well as CO2. The findings highlight the role of chemisorption and subsequent reactions in driving molecular complexity on solid CO, with implications for the chemical evolution of interstellar ices and the potential formation of prebiotic molecules.

2025 ApJ 993 177
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Full-text URL: https://arxiv.org/abs/2509.16978

Interstellar Formation of the Elusive Phosphanyloxyphosphane (H2POPH2) and Phosphanylphosphinous Acid (H2PPHOH) via Nonequilibrium Chemistry: Precursors to the Phosphate Backbone of Nucleotides

Jia Wang, Bing-Jian Sun, Alexandre Bergantini, Zesen Wang, Andrew M. Turner, Agnes H. H. Chang, Ralf I. Kaiser

The P–O–P moiety plays a central role in inorganic and biological systems and is considered to be a critical precursor to the phosphate backbone of nucleotides. However, the isolation of the simplest prototype, phosphanyloxyphosphane (H2POPH2), has remained elusive due to its high susceptibility to hydrolysis. Here, we report the first preparation of phosphanyloxyphosphane and its isomer phosphanylphosphinous acid (H2PPHOH) in low-temperature phosphine (PH3)–carbon dioxide (CO2) ices upon exposure to galactic cosmic ray proxies in the form of energetic electrons. These isomers were isolated and identified in the gas phase using tunable vacuum ultraviolet photoionization reflectron time-of-flight mass spectrometry combined with isotopic labeling studies. Our findings not only suggest that the hitherto undetected phosphanyloxyphosphane and phosphanylphosphinous acid can be synthesized in phosphine-rich extraterrestrial ices but also advance our fundamental understanding of the formation of P–O–P and P–P–O linkages via nonequilibrium chemistry under astrophysical conditions.

J. Am. Chem. Soc. 2025, 147, 43, 38987–38991
DOI: 10.1021/jacs.5c12481
Full-text URL: https://pubs.acs.org/doi/abs/10.1021/jacs.5c12481

Chemical modeling of aminoketene, ethanolamine, and glycine production in interstellar ices

S. Willis, S. Krasnokutski, N. Morin, R. Garrod

Icy interstellar dust grains are a source of complex organic molecule (COM) production, although their formation mechanisms are debated. Laboratory experiments show that atomic C deposited onto interstellar ice analogs can react with solid-phase NH3 to form a CHNH2 radical, a possible precursor to COMs, including aminoketene (NH2CHCO). We used astrochemical kinetics models to explore the role of the reaction of atomic C with NH3 and subsequent reaction with CO in the formation of NH2CHCO and other COMs. We applied the three-phase chemical model MAGICKAL to hot molecular core conditions from the cold-collapse through to the hot-core stage. The chemical network was extended to include NH2CHCO and a range of associated gas-phase, grain-surface, and bulk-ice products and reactions. We also approximated conditions in a shocked cloud, including sputtering of ice mantles. NH2CHCO is formed on grains at low temperatures (~10 K) with a peak solid-phase abundance of ~2e-10 nH. Its formation is driven by nondiffusive reactions, in particular the Eley-Rideal reaction of C with surface NH3, followed by immediate reaction with CO. Surface hydrogenation of NH2CHCO produces ethanolamine with a significant abundance of ~8e-8 nH. In the gas-phase, although ethanolamine reaches a modest abundance peak immediately following its desorption from grains under hot-core conditions, it is destroyed more rapidly due to its high proton affinity. Molecular survival is much higher in the shocked regions, where these species seem most likely to be detected. NH2CHCO is produced efficiently on simulated interstellar grain surfaces, acting subsequently as an important precursor to more complex organics, including ethanolamine and glycine. Ion-molecule gas-phase destruction of NH3-bearing COMs is less efficient in shocked lower-density regions, in contrast to hot cores, enhancing their abundances and lifetimes.

2025, Astronomy and Astrophysics, A27, volume 703
DOI: 10.1051/0004-6361/202554598
Full-text URL: https://arxiv.org/abs/2510.20912

Sense and Sensitivity - I. Uncertainty analysis of the gas-phase chemistry in AGB outflows

M. Van de Sande, M. Gueguen, T. Danilovich, T.J. Millar

Chemical reaction networks are central to all chemical models. Each rate coefficient has an associated uncertainty, which is generally not taken into account when calculating the chemistry. We performed the first uncertainty analysis of a chemical model of C-rich and O-rich AGB outflows using the Rate22 reaction network. Quantifying the error on the model predictions enables us to determine the need for adding complexity to the model. Using a Monte Carlo sampling method, we quantified the impact of the uncertainties on the chemical kinetic data on the predicted fractional abundances and column densities. The errors are caused by a complex interplay of reactions forming and destroying each species. Parent species show an error on their envelope sizes, which is not caused by the uncertainty on their photodissociation rate, but rather the chemistry reforming the parent after its photodissociation. Using photodissociation models to estimate the envelope size might be an oversimplification. The error on the CO envelope impacts retrieved mass-loss rates by up to a factor of two. For daughter species, the error on the peak fractional abundance ranges from a factor of a few to three orders of magnitude, and is on average about 10% of its value. This error is positively correlated with the error on the column density. The standard model suffices for many species, e.g., the radial distribution of cyanopolyynes and hydrocarbon radicals around IRC +10216. However, including spherical asymmetries, dust-gas chemistry, and photochemistry induced by a close-by stellar companion are still necessary to explain certain observations.

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Methylamine Formation on Amorphous Solid Water via the Diffusive CH3 + NH2 Reaction as Investigated by the Cs+ Ion Pickup Method

Arisa Iguchi, Masashi Tsuge, Hiroshi Hidaka, Yasuhiro Oba, Naoki Watanabe

Methylamine (CH3NH2) has been detected in the interstellar media and is considered an important precursor of prebiotic molecules. In addition to gas-phase processes and energetic processing of ice, two nonenergetic pathways have been proposed for the production of CH3NH2 on icy grain surfaces: successive hydrogenation reaction of HCN and CH3 + NH2 reaction. In this work, the latter process was experimentally investigated using the Cs+ ion pickup method, which allowed us to detect reactants (CH3 and NH2) and the product (CH3NH2) in situ. The CH3 and NH2 radicals were produced on amorphous solid water photolyzed by ultraviolet photons, where OH radicals abstracted H atoms from CH4 and NH3, respectively. CH3NH2 was produced even at 10 K, most likely as a result of the transient diffusion mechanism, in which the NH2 radical transiently diffuses a significant distance upon formation to encounter a CH3 radical. During warm-up of samples, the CH3NH2 yield increased between 15–30 K, probably due to the thermal diffusion of CH3 radicals facilitating the CH3 + NH2 → CH3NH2 reaction.

ACS Earth Space Chem. 2025, ASAP Article
DOI: 10.1021/acsearthspacechem.5c00286

Full-text URL: https://pubs.acs.org/doi/10.1021/acsearthspacechem.5c00286

CO adsorption sites on interstellar water ices explored with machine learning potentials: Binding energy distributions and snowline

Giulia M. Bovolenta, Germán Molpeceres, Kenji Furuya, Johannes Kästner, Stefan Vogt-Geisse

Context. Carbon monoxide (CO) is arguably the most important molecule for interstellar organic chemistry. Its binding to amorphous solid water (ASW) ice regulates both diffusion and desorption processes. Accurately characterizing the CO binding energy (BE) is essential for realistic astrochemical modeling. Aims. We aim to derive a statistically robust and physically accurate distribution of CO BEs on ASW surfaces, and to evaluate its implications for laboratory temperature-programmed desorption experiments and interstellar chemistry, with a focus on protoplanetary disks. Methods. We trained a machine-learned potential (MLP) on 8321 density functional theory (DFT) energies and gradients of CO interacting with water clusters of different sizes (22–60 water molecules). The DFT method was selected after extensive benchmarking. With this potential, we built realistic nonporous and porous ASW surfaces and computed a BE distribution. We used symmetry-adapted perturbation theory to rationalize the interactions of CO with the different binding sites. Results. We find that both ASW morphologies yield similar Gaussian-like BE distributions, with mean values near 900 K. However, the nature of the binding interactions is rather different and is critically dependent on surface roughness and dangling OH bonds. Simulated temperature-programmed desorption (TPD) curves reproduce experimental trends across several coverage regimes. From an astrochemical point of view, the application of the full BE distribution has a dramatic influence on the CO distribution in protoplanetary disks, leading to a broader CO snowline region, improving predictions of CO gas-ice partitioning, and suggesting an equally broader distribution of organics in these objects.

A&A, 703 (2025) A172
DOI: 10.1051/0004-6361/202555836
Full-text URL: https://arxiv.org/abs/2508.14219

Computational and Spectroscopic Investigation of Diaminomethane Formation: The Simplest Geminal Diamine of Astrochemical Interest

Pravi Mishra, Parmanand Pandey, Rachana Singh, Manisha Yadav, Shivani, Aftab Ahamad, Alka Misra, Amritanshu Shukla and Poonam Tandon

A high-level ab initio characterization and formation of diaminomethane (DAM), the simplest geminal diamine, is presented to support its spectroscopic detection and astrochemical relevance in the interstellar medium. The C2v DAM conformer is identified as the global minimum, while C1 DAM and C2 DAM represent higher-energy local minima. The proposed reaction pathways are exothermic and proceed without activation barriers. Simulated infrared spectrum reproduces accurate key spectral signatures with several vibrational modes exhibiting strong IR intensities (>80 km mol−1), particularly in the 800–3000 cm−1 range and band shapes. Dipole moments and accurate rovibrational spectroscopic parameters, including rotational constants, anharmonic vibrational frequencies, quartic and sextic distortion constants, and nuclear quadrupole coupling constants are reported to assist with high-resolution spectroscopic identification. This study provides significant theoretical benchmarks for its formation and offers guidance for future laboratory spectroscopy and molecular searches in interstellar environments.

Atoms 2025, 13(11), 91
DOI: 10.3390/atoms13110091
Full-text URL: https://doi.org/10.3390/atoms13110091

Announcements

Professor in Planetary Sciences / University of Bern, Switzerland

The Division of Space Research and Planetary Sciences of the Physics Institute, University of Bern, Switzerland, invites applications for a full-time position as a Professor in Planetary Sciences. The initial level of tenure can range from assistant professor tenure track to full professor depending on qualifications (open rank). We invite applications from candidates who conduct outstanding research, teaching, mentorship, and leadership in any area of experimental planetary science. Areas of research could include, but are not limited to, the properties, origin and evolution of planets and minor bodies in the Solar System, the search for and emergence of life beyond Earth, the composition of surfaces and atmospheres, ongoing physical and chemical surface and sub-surface processes and the evolution of planetary interiors. A diverse spectrum of approaches and methodologies is welcome, including, but not limited to, the analysis and modeling of space probe datasets, instrumentation and flight hardware development, experimental, observational and laboratory techniques, comparative planetology or the involvement, development and leadership in space missions.
The full announcement can be found here: https://ohws.prospective.ch/public/v1/jobs/5910a4be-30c9-4e9d-abbe-9bc44b71776e

COSPAR Scientific Assembly 2026, Scientific Event F3.4: "Interstellar Chemistry, Interstellar Origins: Observations, Experiments, Models and Theory of the Molecular Evolution of the Universe."

Organizers Rob Garrod and Sergio Ioppolo invite submissions for contributed talks and posters at their COSPAR 2026

Scientific Event F3.4: "Interstellar Chemistry, Interstellar Origins: Observations, Experiments, Models and Theory of the Molecular Evolution of the Universe." COSPAR (Committee on Space Research) is a large international organization that sponsors scientific assemblies about space research, with their main Scientific Assembly held every other year.

The 46th COSPAR Scientific Assembly will be held in Florence, Italy from 1–9 August 2026, and will be a fully in-person meeting. The F3.4 sessions are expected to comprise a total of two days-worth of talks, and there will be ample capacity for poster presentations. The event description and confirmed speakers are given below. We especially encourage early-career speakers to submit abstracts for both oral and poster presentations. Abstracts may be submitted on the assembly web page (https://www.cospar-assembly.org) by going to "Abstract Submission" and "Log-in".

Abstract submission opens Nov. 8 2025, closing Feb. 13, 2026.

A selection of refereed papers from the event will be published in Advances in Space Research or Life Sciences in Space Research, and authors are encouraged to submit manuscripts after the Assembly for consideration. Details about the scientific program, transportation, financial aid, and logistics can be found at the above website, and at the local website https://cospar2026.org. A number of interesting scientific sessions will take place during the conference, including others with astrochemistry-related topics. The "Call for Abstracts" document (PDF) contains various information about COSPAR 2026, and can be downloaded here: https://cospar2026.org/wp-content/uploads/2025/08/Call-for-Abstract.pdf.

Questions about our session F3.4, or COSPAR 2026 more generally, can be addressed to Rob Garrod (rgarrod@virginia.edu) and/or Sergio Ioppolo (s.ioppolo@phys.au.dk).

We look forward to reading your abstracts and to seeing you in Florence next year!

Event Description:
Molecular observations from centimeter to infrared wavelengths continue to show the richness of interstellar chemistry. Data from JWST now indicate the presence of both simple and highly complex organic species in dust-grain ice mantles, as well as probing molecular distributions in the hot gas close to protostars. The now mature ALMA telescope continues to drive our understanding of gas-phase chemistry in star and planet-forming sources. As the observational knowledge-base has grown, experimental, computational and theoretical astrochemistry research has risen to the challenge to interpret this new data. This Event will gather researchers in all areas of astrochemistry with interests in molecular evolution and complexity and the earliest origins of life. We will provide a platform for young researchers, especially those from developing countries, to present their work to an international audience.
Scientific Organizing Committee:
Rob Garrod, Main Scientific Organizer (University of Virginia, USA)
Sergio Ioppolo, Deputy Scientific Organizer (Aarhus University, Denmark)
Olivier Berné (IRAP, Toulouse, France)
Jordy Bouwman (University of Colorado, Boulder, USA)
Stefano Bovino (Universidad de Concepción, Chile)
Paola Caselli (Max Planck Institute for Extraterrestrial Physics, Germany)
Claudio Codella (INAF - Osservatorio Astrofisico di Arcetri, Florence, Italy)
Jennifer Noble (Aix-Marseille University, France)
Cristina Puzzarini (University of Bologna, Italy)
Albert Rimola (Universitat Autònoma de Barcelona, Spain)

Confirmed Speakers:
Eleonora Bianchi (INAF Florence, Italy)
Ewen Campbell (University of Edinburgh, Scotland)
Joan Enrique-Romero (Leiden University, Netherlands)
Brandt Gaches (Chalmers University, Sweden)
Tommaso Grassi (MPR, Germany)
Liv Hornekaer (Aarhus University, Denmark)
Helgii Hrodmarsson (Universite Paris Est Creteil, France)
Thanja Lamberts (Leiden University, Netherlands)
Niels Ligterink (Delft University of Technology, Netherlands)
Belén Maté (Consejo Superior de Investigaciones Científicas, Spain)
Anna Miotello (ESO, Germany)
Els Peeters (University of Western Ontario, Canada)
Alexey Potapov (University of Jena, Germany)
Olli Sipilä (MPE, Germany)
Zac Smith (Leiden University, Netherlands)
Gabi Wenzel (MIT, USA)

Tenure-Track Faculty in Astronomy and Astrophysics University of Georgia / Department of Physics and Astronomy

The Department of Physics and Astronomy at the University of Georgia invites applications for a tenure-track position at the rank of Assistant or Associate Professor in observational astronomy and astrophysics, with an anticipated start date of

August 2026. We welcome applicants at both ranks, with encouragement for early-career scientists at the Assistant Professor level.
We are especially interested in candidates whose research focuses on young stars, exoplanets, circumstellar disks (protoplanetary, transitional, or debris), or planetary sciences. However, exceptional candidates in all areas of observational, computational, or theoretical astronomy and astrophysics will be considered. Applicants must hold a Ph.D. in astronomy, physics, or a closely related field and have at least one year of postdoctoral experience. The successful candidate is expected to establish a vigorous, externally funded research program, contribute to high-quality teaching and mentoring at both undergraduate and graduate levels, and engage in interdisciplinary collaboration.
The Department of Physics and Astronomy currently includes 20 faculty members, including 3 in astronomy and astrophysics. Our faculty maintain active collaborations with colleagues in Chemistry, Geography, Geology, and Statistics. Astronomy faculty are frequent users of major ground- and space-based observatories, including ALMA, ARO, JWST, Gemini, Keck and XRISM. Departmental resources include the UGA Observatory, the Center for Simulational Physics, and the Quantum Networks Training and Research Alliance in the Southeast.
Applicants should only apply at https://www.ugajobsearch.com/postings/458945. Applicants should prepare the following application documents: (1) a cover letter with brief summaries of their scientific background, strengths, plans, and teaching experience; (2) a complete curriculum vitae; (3) a statement of research interests, philosophy, and plan (3 page maximum); (4) a description of teaching philosophy and mentoring plans (2 page maximum); and (5) contact information only for three references. References will be contacted later in the search process, but applicants are strongly encouraged to pre-arrange with references for letters of recommendation.
Any other correspondence should be addressed to the search committee chair, Prof. Inseok Song (song@uga.edu). All applications received by December 31, 2025 will receive full consideration, but review will continue until the position is filled.
The Franklin College of Arts and Sciences is the heart of UGA's learning environment, advancing knowledge, research, and creative activity across more than 40 departments, schools, and institutes. With a vision for high-impact research and education, Franklin College prepares students for leadership and global engagement in a sustainable future. The Department and the College have a strong commitment to multidisciplinary research, collaboration, and academic innovation.
Chartered by the state of Georgia in 1785, the University of Georgia is the birthplace of public higher education in America and is the state's flagship university (https://www.uga.edu/). The proof is in our more than 240 years of academic and professional achievements and our continual commitment to higher education. UGA is currently ranked among the top 20 public universities in U.S. News & World Report. The University's main campus is located in Athens, approximately 65 miles northeast of Atlanta, with extended campuses in Atlanta, Griffin, Gwinnett, and Tifton. UGA employs approximately 3,100 faculty and more than 7,700 full-time staff. The University's enrollment exceeds 41,000 students including over 31,000 undergraduates and over 10,000 graduate and professional students. Academic programs reside in 19 schools and colleges, including our newly established School of Medicine.
The University of Georgia is an Equal Opportunity employer. All qualified applicants will receive consideration for employment without regard to age, color, disability, genetic information, national origin, race, religion, sex, or veteran status or other protected status. Persons needing accommodations or assistance with the accessibility of materials related to this search are encouraged to contact Central HR (hrweb@uga.edu).

Call for papers, Special Issue on Planetary and Space Science "Planetary Simulants: experiments as a tool for remote sensing and in-situ exploration"

Simulants are necessary tools to interpret data of planetary surfaces. Their production and characterization is mandatory to shed light on the properties of surfaces and atmospheres and to design future exploration.

Understanding the bodies of the Solar System benefits from the development and use of planetary simulants, samples prepared to realistically replicate the physical, chemical, mechanical, and spectral properties of planetary surfaces and atmospheres.

Simulants play a crucial role in planetary science: their controlled and reproducible properties allow researchers to interpret remote sensing and in situ data, develop and test mission hardware, optimize sampling strategies, and refine mobility and landing protocols. Additionally, simulants offer a consistent experimental baseline across laboratories, promoting reproducibility and enabling comparative studies.

This special issue of Planetary and Space Science invites contributions that advance our knowledge of planetary surfaces and atmospheres/exospheres through the use of laboratory simulants. We welcome manuscripts presenting experimental studies, data analysis, and modeling of laboratory data using simulants across a wide range of techniques.
Submission deadline: 31 March 2026

For more details see https://www.sciencedirect.com/special-issue/10J1416J3BJ

PhD and PostDoc Opportunities at the University of Bern: Exploring Abiotic Organic Complexity

The Space Research and Planetary Sciences Division at the University of Bern is offering two PhD positions and one PostDoc position focused on analysing legacy data from ESA's Rosetta mission to comet 67P/Churyumov–Gerasimenko. These positions are dedicated to the data-driven investigation of cometary abiotic organic complexity (AOC) based on highly convolved high-resolution mass spectra, with the goal of developing a reference framework for future space missions, including those searching for signs of extraterrestrial life. Working within an interdisciplinary team that combines astrobiology with analytical chemistry (namely, mass spectrometry) and data science, successful candidates will systematically inventory prebiotic molecular signatures or develop data-analysis pipelines that integrate chemometrics/multivariate statistics and

scientific machine learning to enable an unbiased, data-driven characterization of cometary AOC.
Detailed information can be found at the following links:
PhD1: https://ohws.prospective.ch/public/v1/jobs/33cb65f1-1d68-42ba-95fa-4fb7d14e3cbc
PhD2: https://ohws.prospective.ch/public/v1/jobs/69f82d6b-7faf-4333-9ac3-1793815f8681
PostDoc: https://ohws.prospective.ch/public/v1/jobs/fd6375b0-855d-4643-9f63-f74e3406bef7

PhD position in laboratory astrochemistry

A PhD position entitled “Laboratory studies of the processing of astrochemical ices” is available for September 2026 in Professor Wendy Brown’s research group at the University of Sussex, UK. Prospective applicants should have a qualification in Chemistry, Physics or a related discipline.
The position will be funded from an EPSRC DLA award to the University of Sussex. This is an open competition across the University and there will be 10 PhD positions funded in total. Applications are open to UK and overseas PhD candidates.
Here you can find a link to the projects and to the application process for the EPSRC funded positions:
https://www.sussex.ac.uk/study/fees-funding/phd-funding/view/1868-EPSRC-Science-and-Engineering-studentships
The brochure detailing all available projects, including this one, can be found by following the link from that website.
As part of this PhD position, there will also be a 2-3 months research placement at the FELIX laboratory at Radboud University in Nijmegen in The Netherlands. The accommodation costs for the time in The Netherlands will be funded by the FELIX laboratory. Please contact Wendy Brown (w.a.brown@sussex.ac.uk) if you would like any further information.
The application deadline is January 6th 2026.