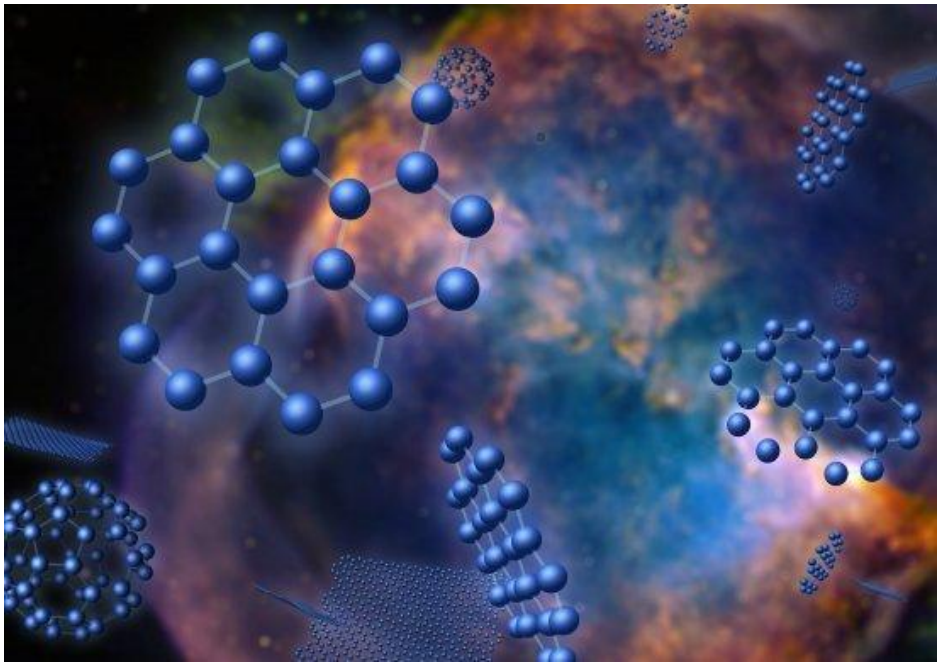
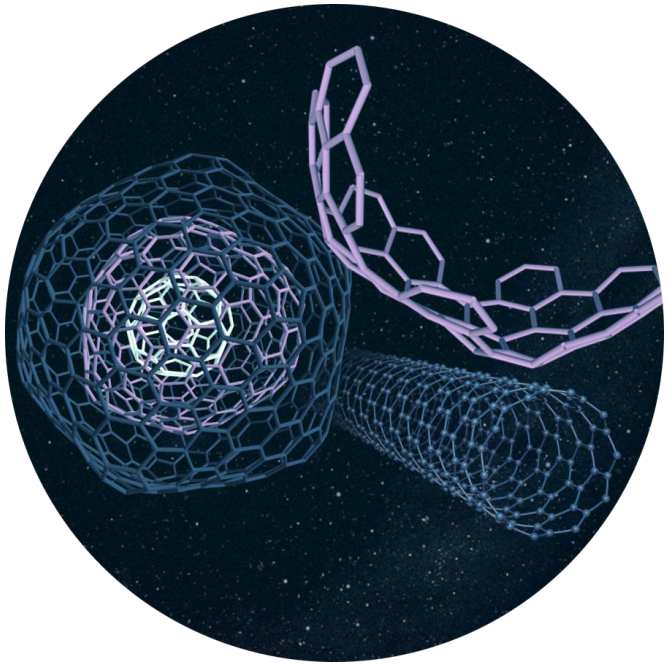
NanoSpace and AI in Astrochemistry TS overview

The case of carbon chemistry around old stars





Domingo Aníbal García Hernández

Funded by the European Union

CA 21126
01/11/2022 - 31/10/2026

AI in Astrochemistry Training School
05/08/2025



NanoSpace

Carbon molecular nanostructures in space

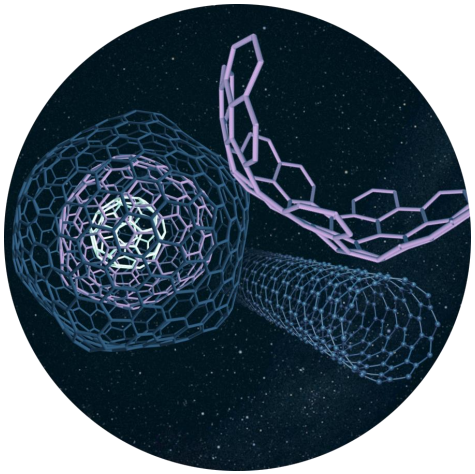


Domingo Aníbal García Hernández

cost
EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

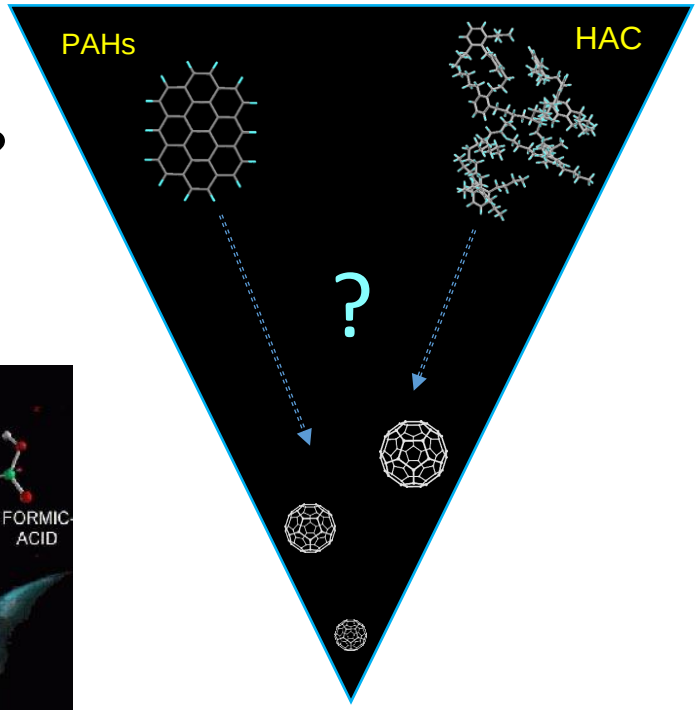
Funded by the European Union

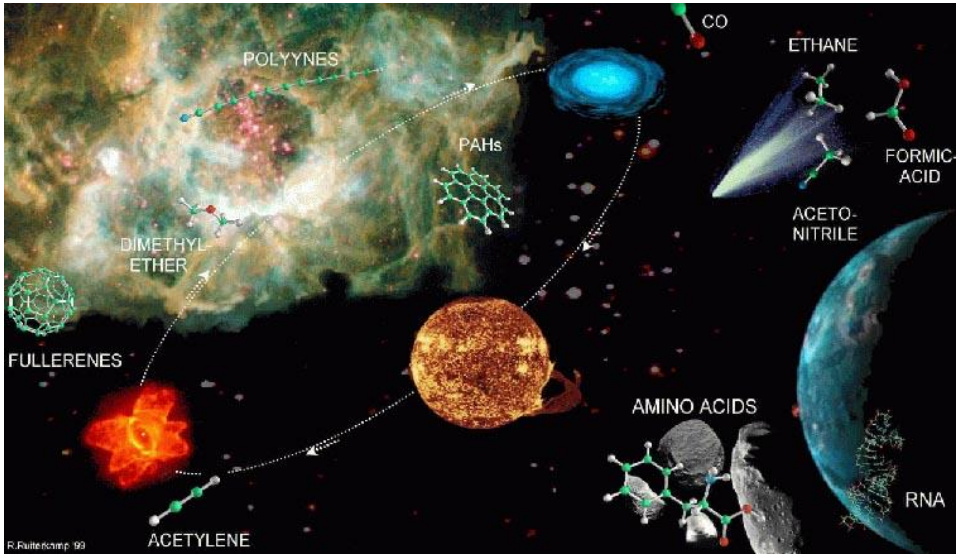
Key scientific challenges



SC1: nC species?

SC2: Chemical pathways?

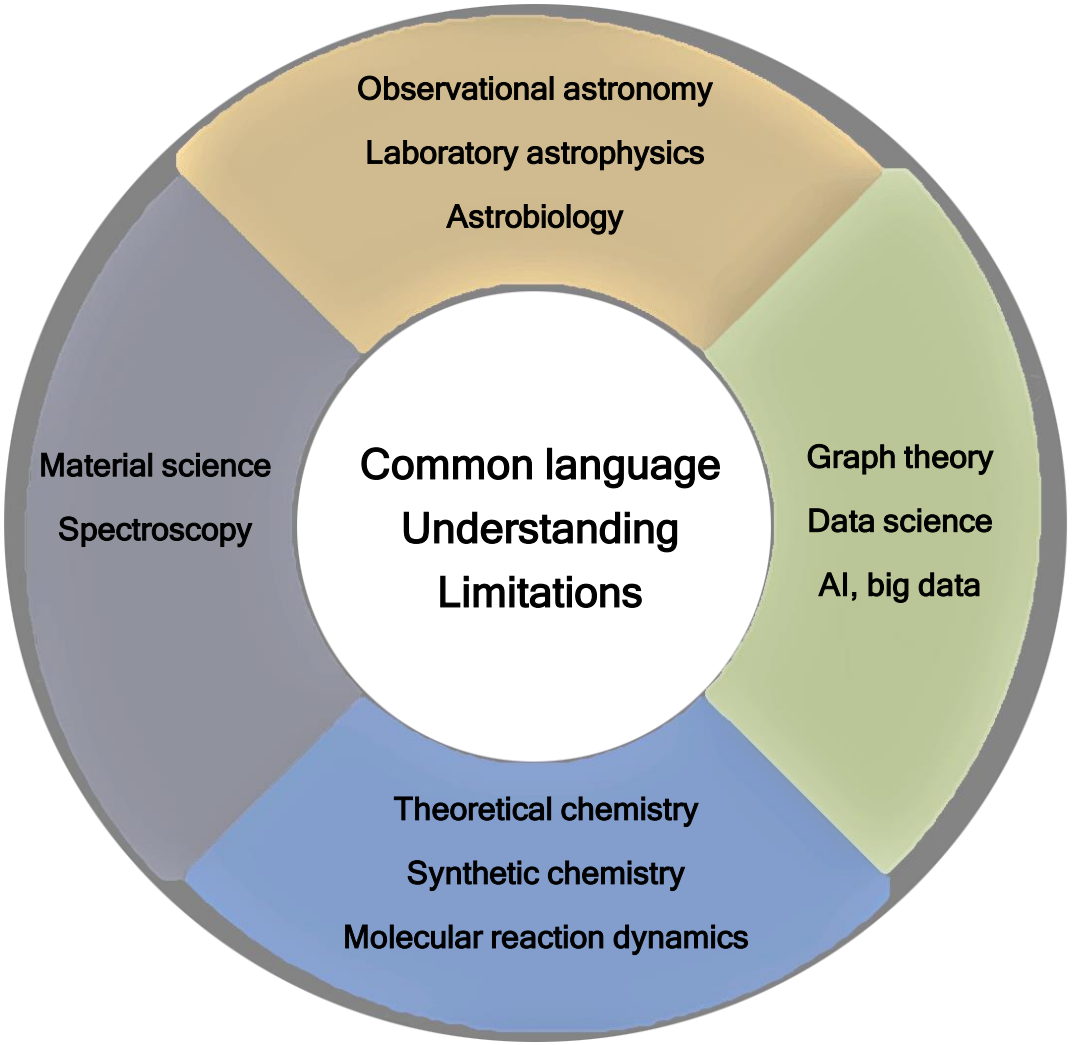




SC3: nC role?

NanoSpace

Interdisciplinary approach



International Participation



NanoSpace mailing list & Media

nanospace@iac.es

MAILING LIST

@COSTNanoSpace

slack

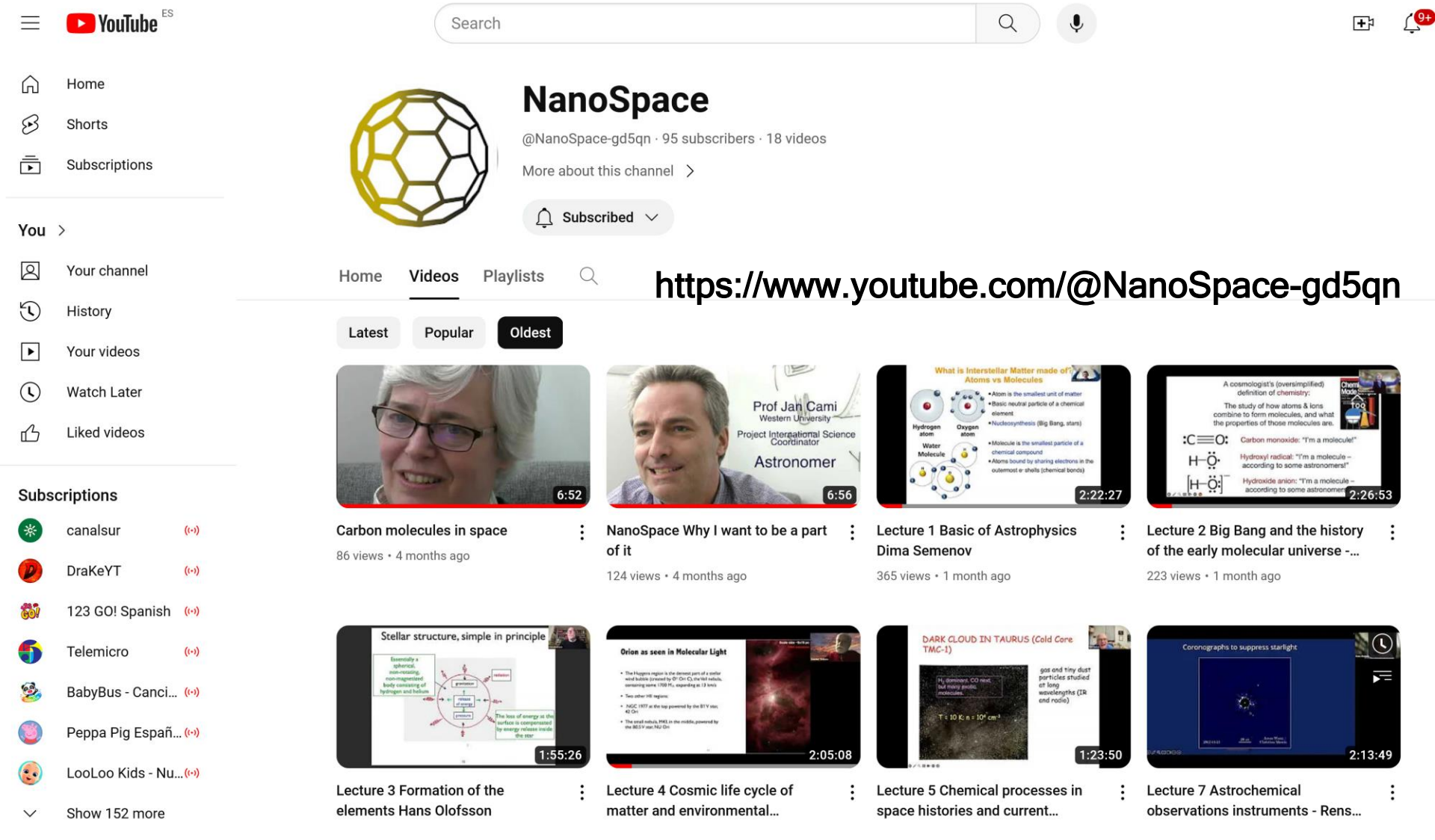
COST NanoSpace

LinkedIn

NanoSpace - COST



NanoSpace YouTube Channel



IAC Action Website

NanoSpace

Carbon molecular nanostructures in space

https://research.iac.es/proyecto/nanospace/

HOME

PARTICIPANTS AND WORKING GROUPS

- Participants
- Working Groups

MOBILITY GRANTS

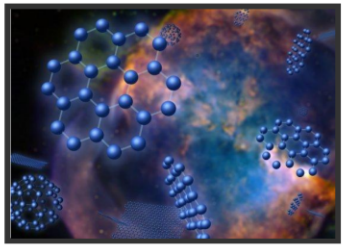
- STSMs
- Funded STSMs
- ITC Conference Grants
- Funded ITC Conference Grants
- YRI Conference Grants

EVENTS

- Joint Scientific Meetings
- Training Schools
- Online Webinars/Lectures
- Working Group Meetings

The main aim and objective of the COST Action NanoSpace ("Carbon molecular nanostructures in space"; CA21126) is to advance the fundamental understanding of the physics and chemistry of cosmic carbon nanomaterials (nanocarbons; nC) and their relevance in non-terrestrial environments by promoting the interdisciplinary combination of state-of-the-art astronomical, laboratory, and theoretical studies, among others.

General Action Scope



The main scientific challenges are the following:

- What nanocarbon species are present in space and how can we identify them?
- What are the chemical pathways that lead to their formation and destruction?
- What is the role of nanocarbon species in non-terrestrial environments? This is in cosmic and in prebiotic chemistry (astrobiology) and in astrophysics.

In order to attack the scientific challenge, NanoSpace proposes an interdisciplinary approach, combining the expertise from a wide range of disciplines like observational astronomy, laboratory astrophysics, astrobiology, theoretical chemistry, synthetic chemistry, molecular reaction dynamics, material science, spectroscopy, graph theory, and data science (AI, big data). The ambitious interdisciplinary nature of NanoSpace has the advantage that nanocarbons have potential applications in nanotechnology. Researchers and innovators from all these fields are thus welcome to participate in the Action as Working Group members, applying here .

NanoSpace takes advantage of the recent successful operation of the James Webb Space Telescope (JWST), the new facilities that can better mimic the interstellar medium (ISM) on the ground as well as the recent developments in the computational facilities and in laboratory techniques.

Joint and WG meetings



1st COST NanoSpace Joint Scientific Meeting

February 9th - 11th, 2023, Ljubljana (Slovenia)

1st COST NanoSpace Joint Scientific Meeting

Book of abstracts



2nd COST NanoSpace Joint Scientific Meeting

April 16th - 19th, 2024, Istanbul (Turkey)

2nd COST NanoSpace Joint Scientific Meeting

Book of abstracts



3rd COST NanoSpace Joint Scientific Meeting

May 13th - 16th, 2025, Kaunas (Lithuania)

3rd COST NanoSpace Joint Scientific Meeting



NanoSpace Working Group 2 Meeting: "Processing, reactivity and relaxation pathways of nC"

February 20th - 23th, 2024, Edinburgh (Scotland, UK)

1ST MEETING OF NANOSPACE WORKING GROUP 2

Book of abstracts



NanoSpace Working Group 1/4 Meeting: "NanoteC24 - Carbon nanoscience and nanotechnology"

August 27th – 30th, 2024, Nantes (France)

NanoteC24 - Carbon nanoscience and nanotechnology

Book of abstracts



NanoSpace Working Group 4 Meeting: "Cardiff WG4 NanoSpace Hackathon"

January 21st - 24th, 2025, Cardiff (United Kingdom)

Cardiff WG4 NanoSpace Hackathon

WG4 Meeting Report









Training Schools

COST NanoSpace JWST Training School



NanoSpace Astrochemistry Training School



COST NanoSpace AI in Astrochemistry Training School



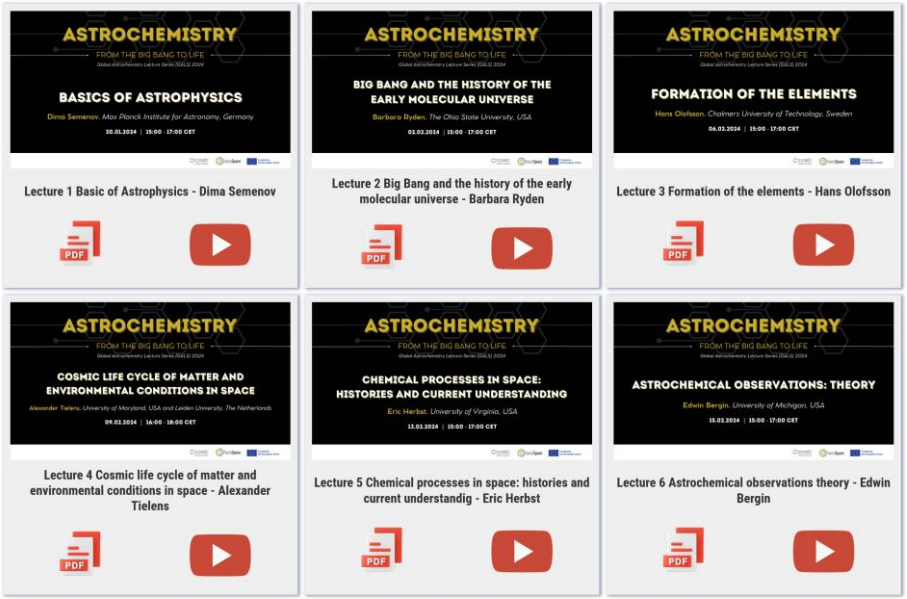
On-line Lectures

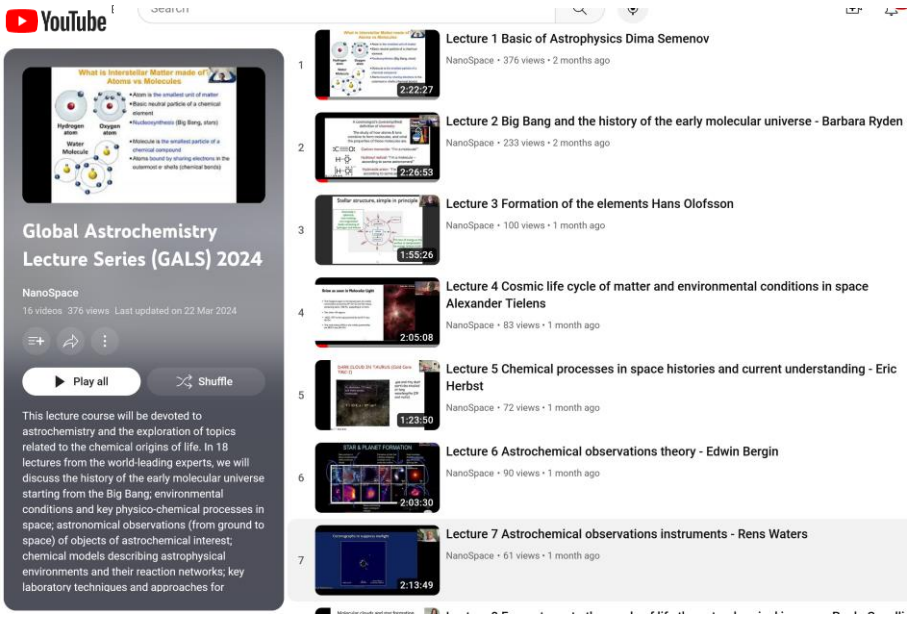


- 340 participants; ~100 per lecture
- Credit weighting of 3 ECTS
- Accredited by Faculty of Sciences, ULL

ORGANIZERS

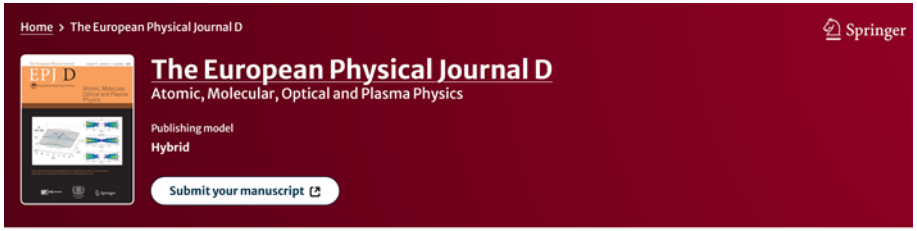
Robin Garrod	Wolf Geppert	Serge Krasnokutski	Martin McCoustra	Alexey Potapov (Chair)
University of Virginia, USA	Stockholm University, Sweden	Friedrich Schiller University Jena, Germany	Heriot-Watt University, Scotland	Friedrich Schiller University Jena, Germany





Some Action updates

Preliminary Roadmap already in press in EPJD



Database work and on-line Database Strategy Group meetings (already started)



On-line WG1-4 meetings and Webinars (already initiated)

WG2 NanoSpace Webinar

30 April 2025 13:00-14:00 CEST

Ion-molecule collision experiments still exist and they can be useful
Sylvain Maclot
University of Caen Normandy (France)



Laboratory IR ice spectroscopy for the interpretation of JWST observations
Jennifer Noble
CNRS PIIM Marseille (France)



WG2 NanoSpace Webinar

12 March 2025 13:00-14:00 CET

Carbon structures & synchrotron radiation: what can be done at SOLEIL
Alexandre Giuliani
Synchrotron SOLEIL, Saint-Aubin, France



PAH and fullerene studies at DESIREE
Michael Gatchell
Department of Physics, Stockholm University, Sweden



Enjoy NanoSpace and participate

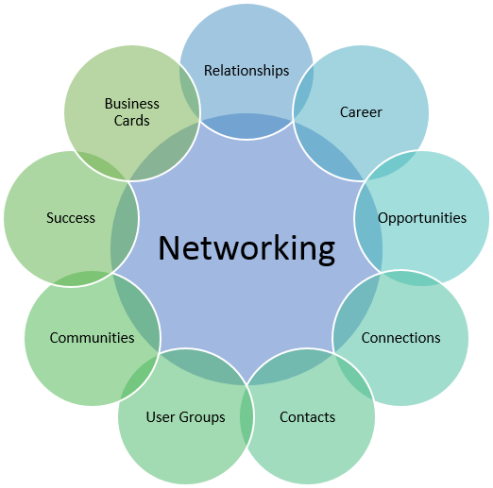
Collaborate



Participate / lead



Benefit



Action databases/deliverables:

- Expertise
- Lab facilities
- Nanocarbon properties
- ….

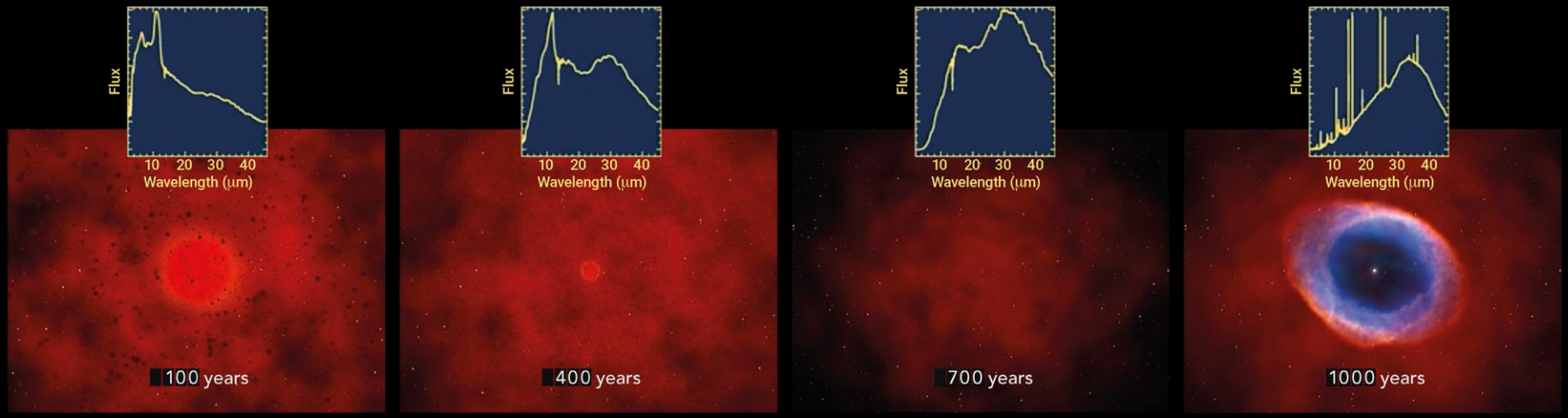
Action events/tasks:

- Scientific meetings
- Training Schools
- Outreach
- ….

Networking activities:

- Scientific exchange
- Learning/Training
- Grants (STSMs, ITC, etc.)
- ….

Complex carbon chemistry around old stars
AI/ML avenues



C_3, C_2H_2, HCN,…

PAHs, C_{60}, UIRs

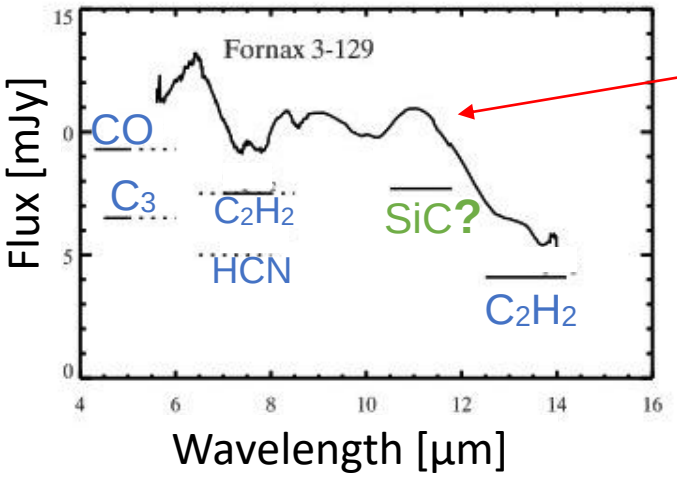
Unidentified solid-state C compounds (UIRs)

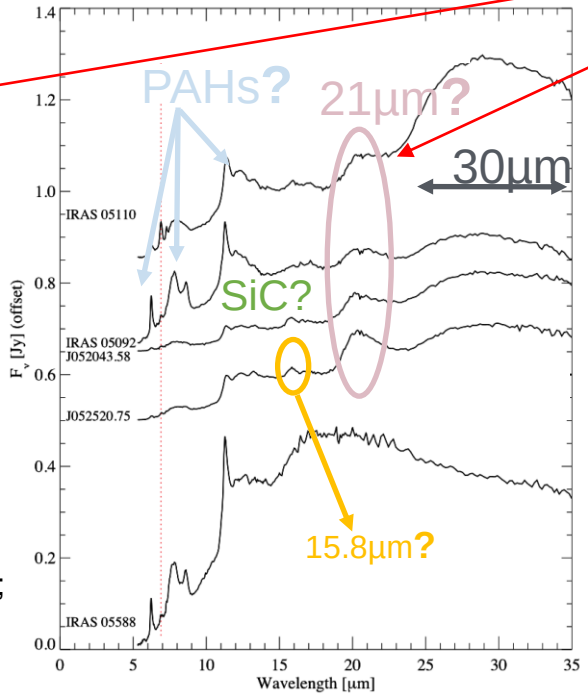


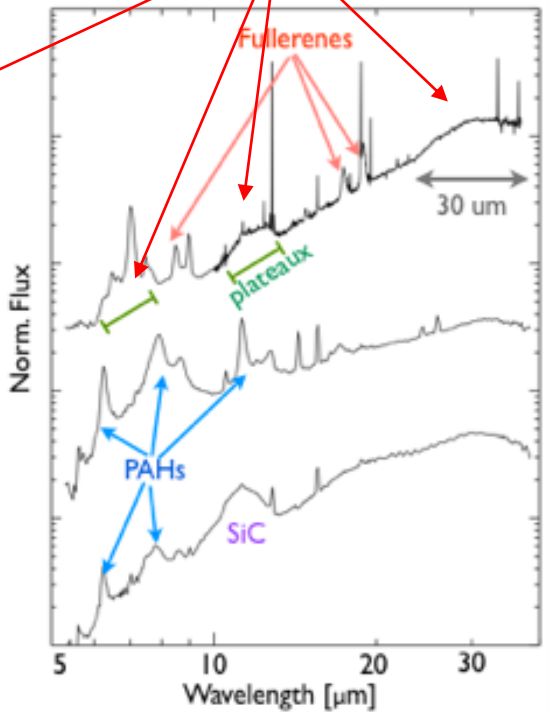
Why do we study old stars?

Complex nanocarbons in old stars

Solid-state UIR features



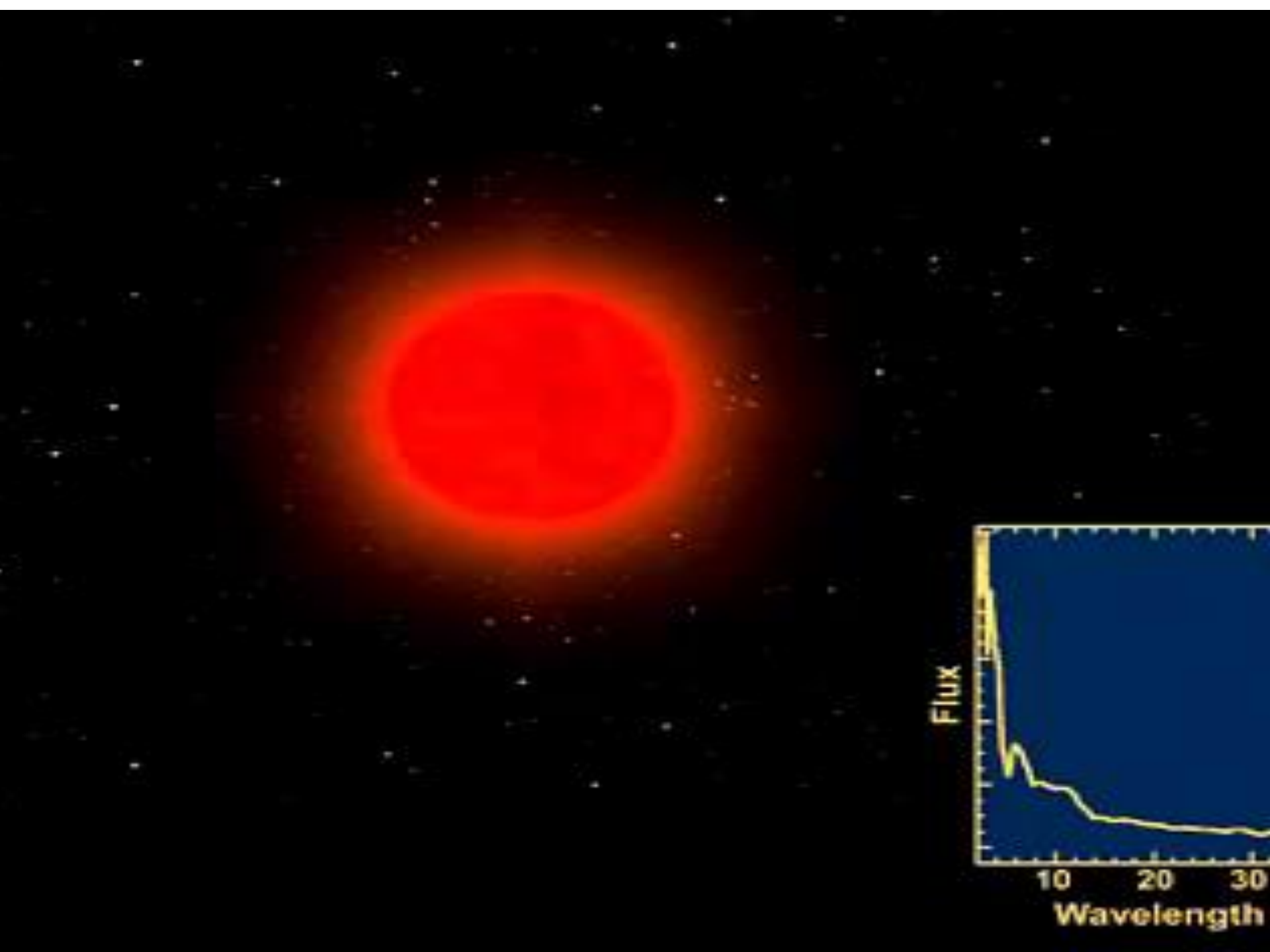




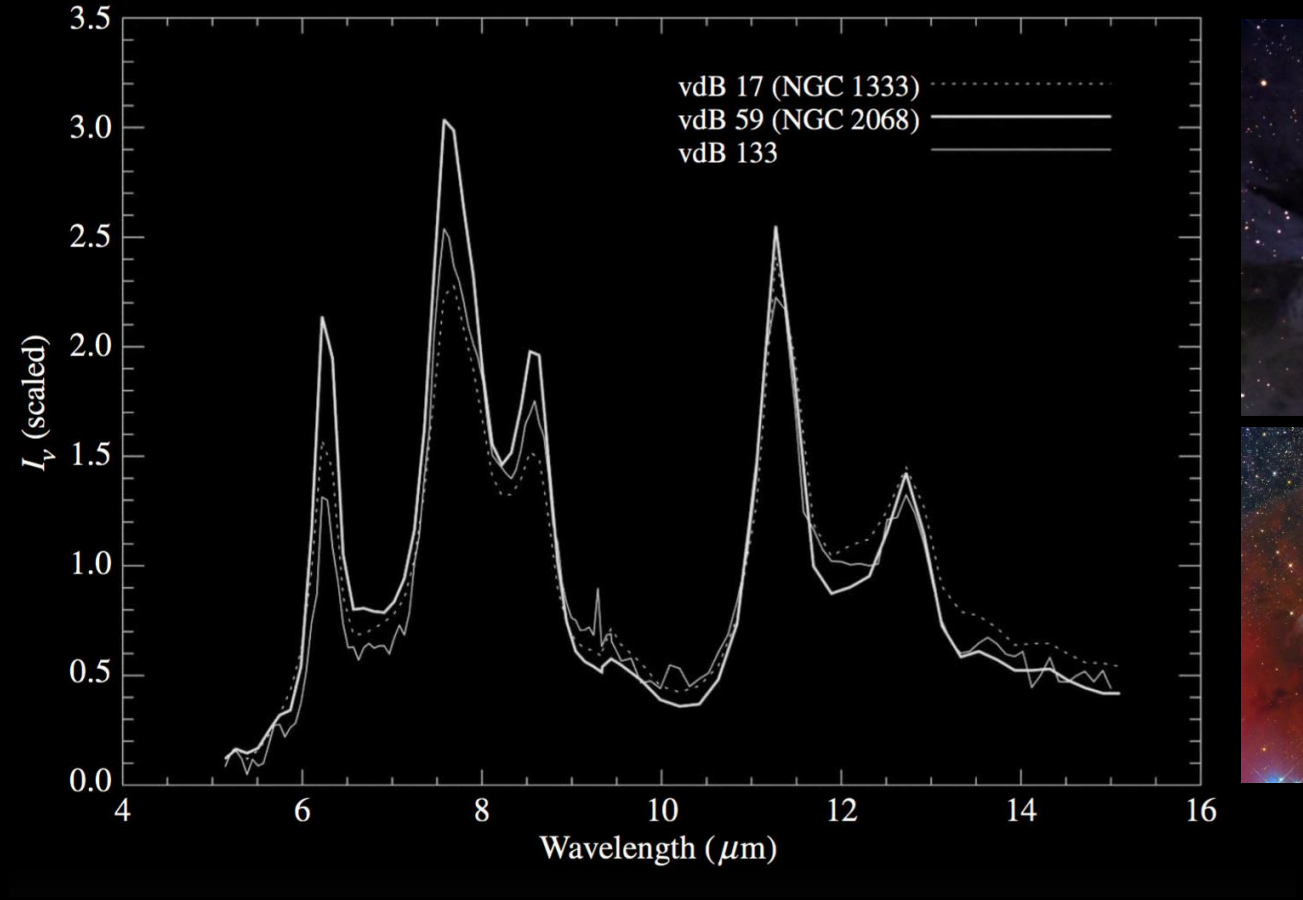
Matsuura et al. (2007,2014), Sloan et al. (2014); Bernard-Salas et al. (2012)

AGBs | Post-AGBs | PNe

Organic diversity + objects simplicity + short timescale = best laboratory in space


Flux
10
20
30
Wavelength

UIR'S ORIGIN?



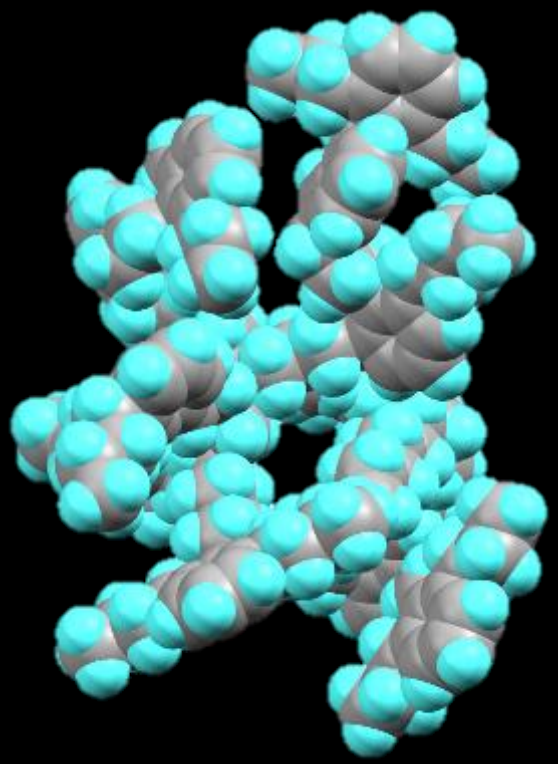




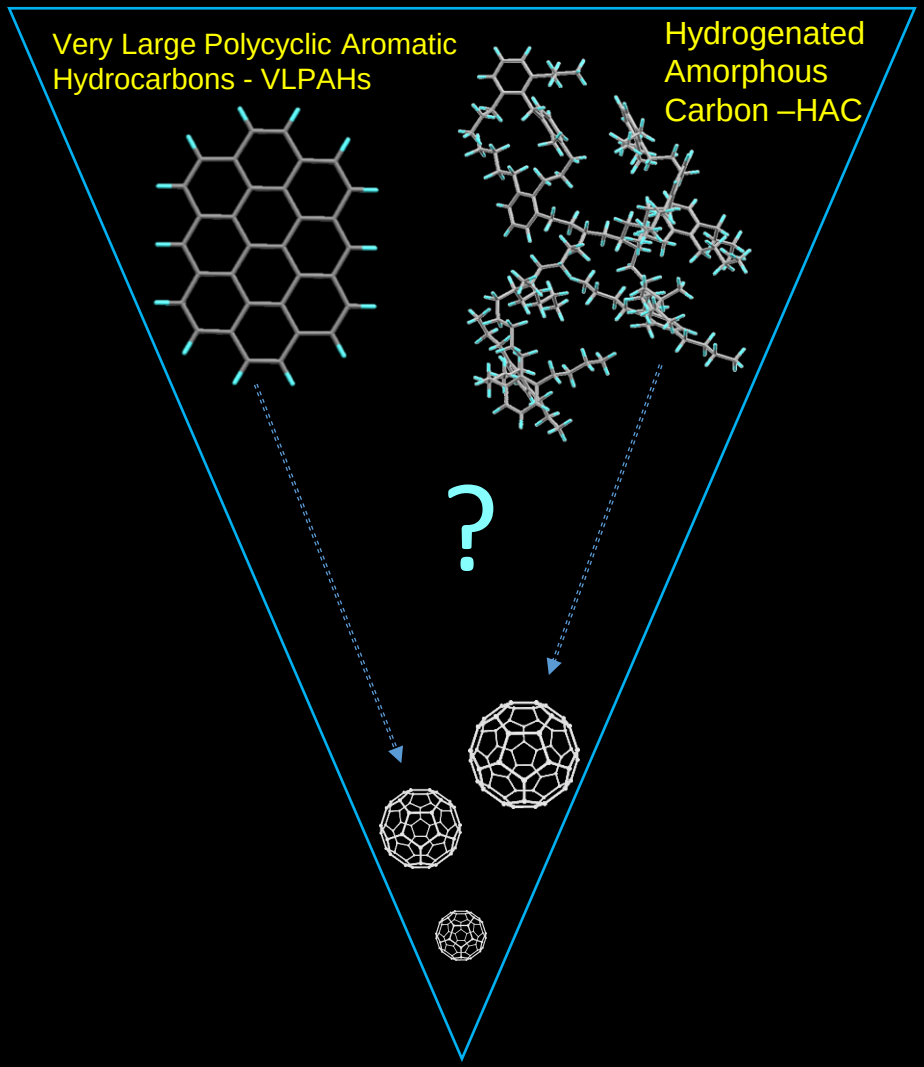
Unidentified InfraRed emission – UIR

FORMATION ROUTES?

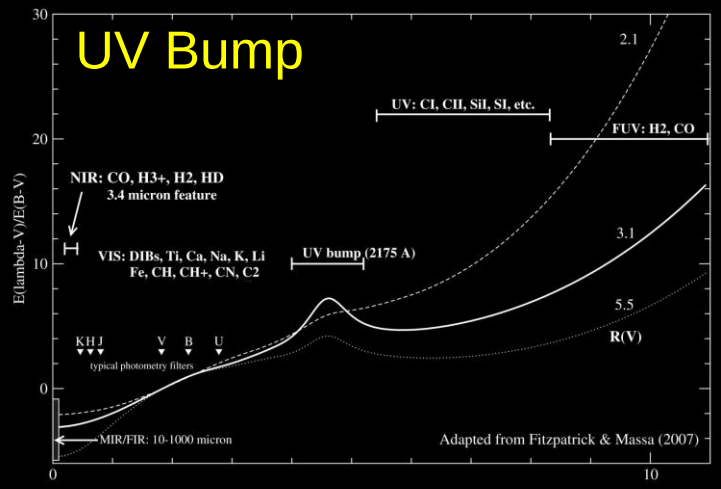
3D structures



Top-down chemistry

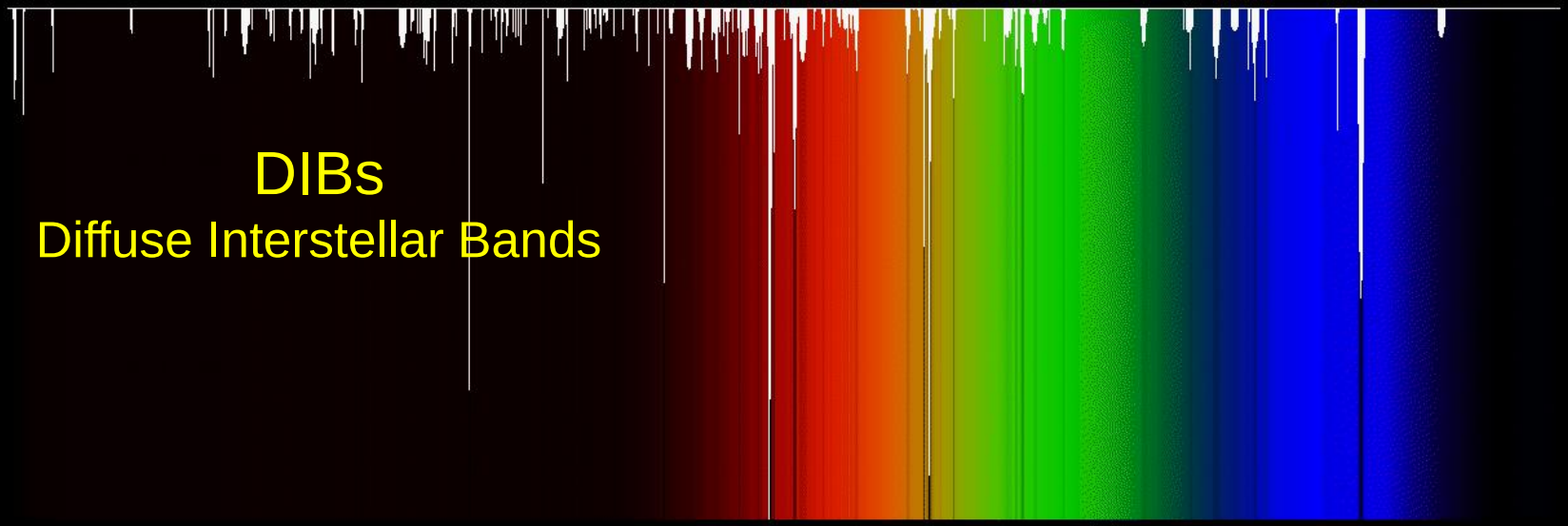


ASTROCHEMISTRY ROLE?





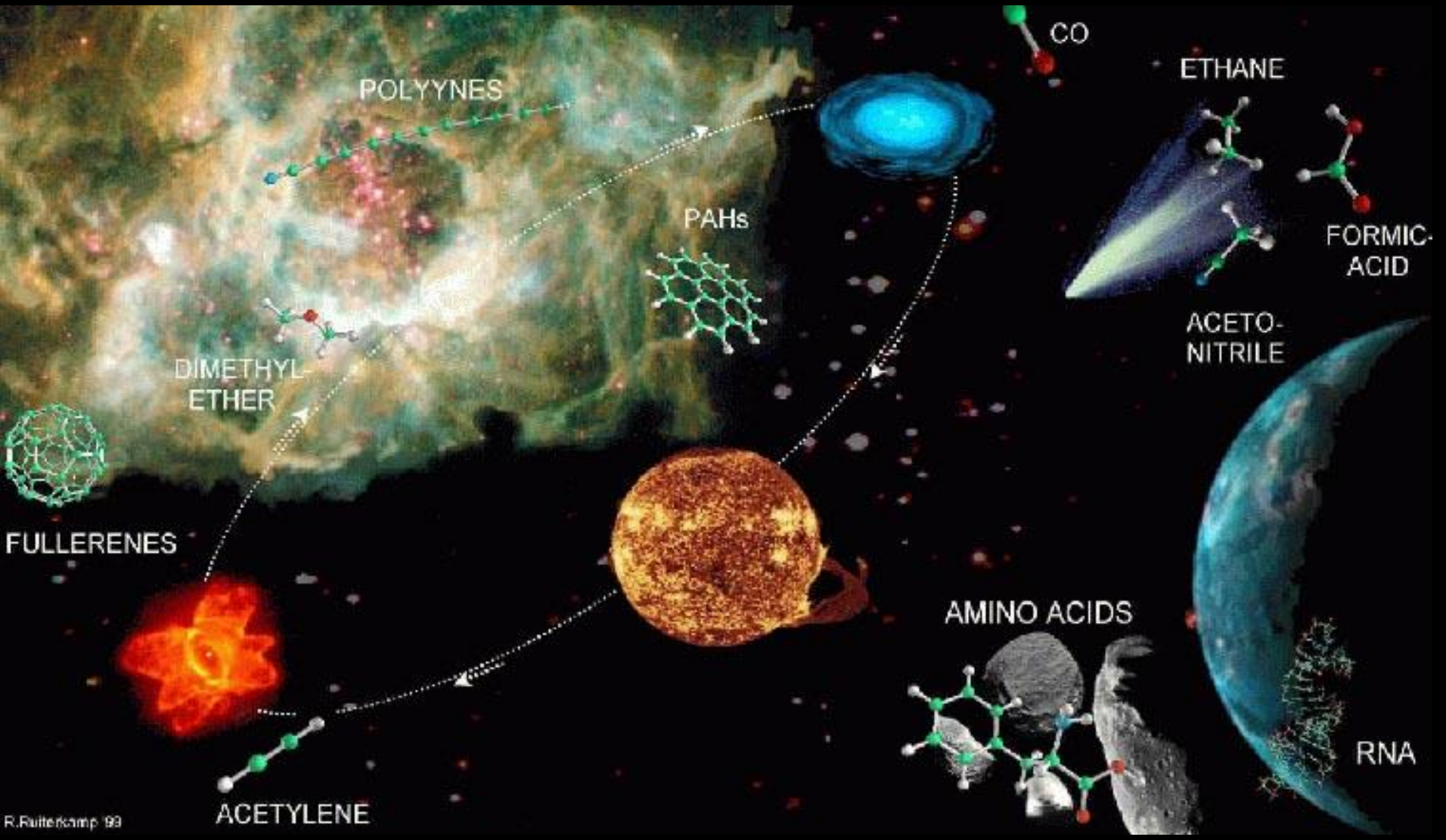




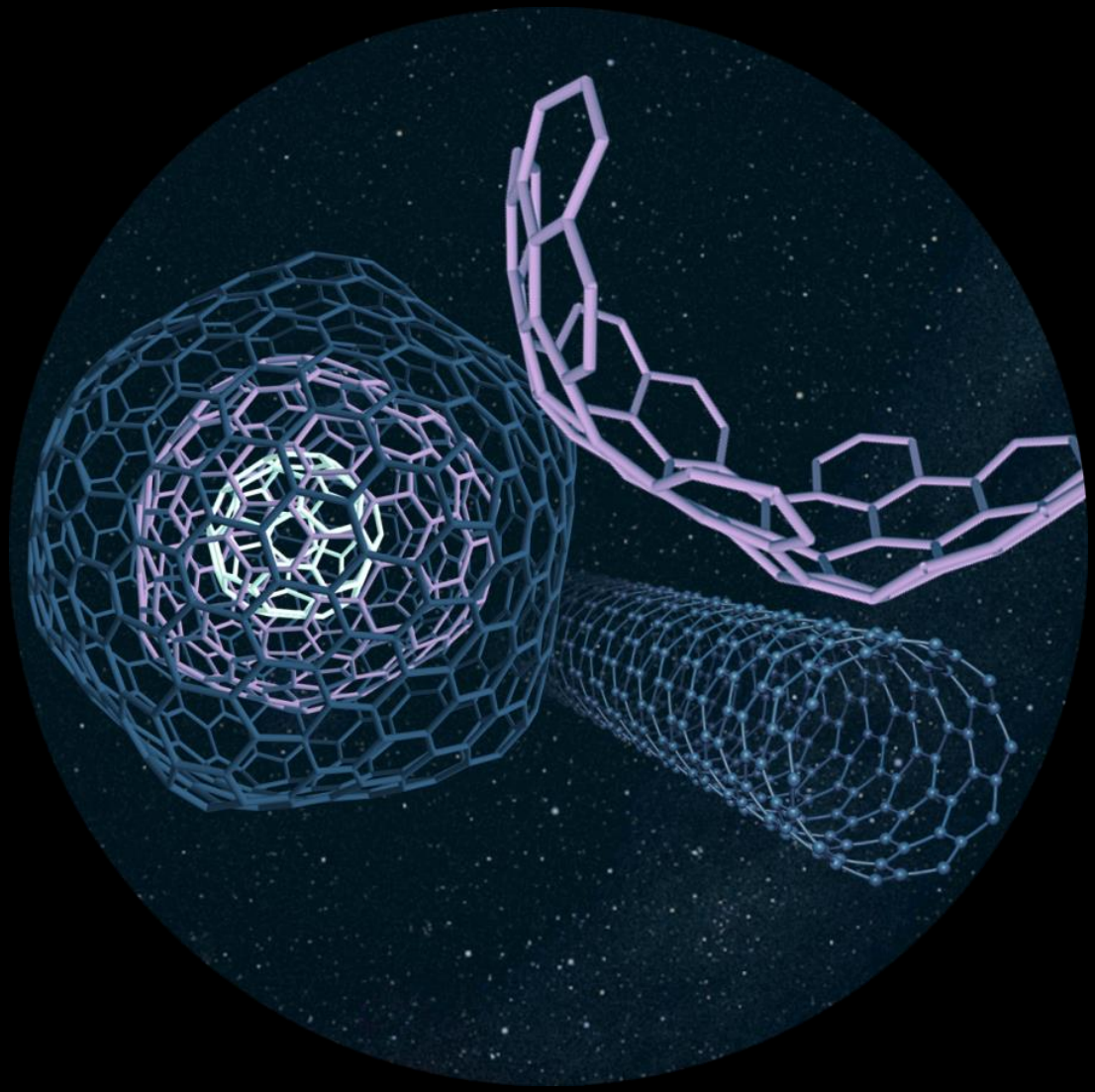
DIBs

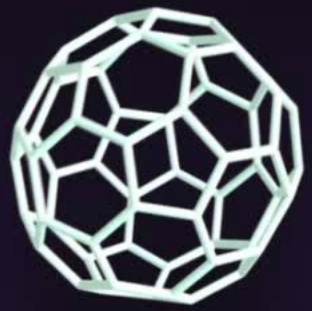
Diffuse Interstellar Bands

ASTROBIOLOGY ROLE?



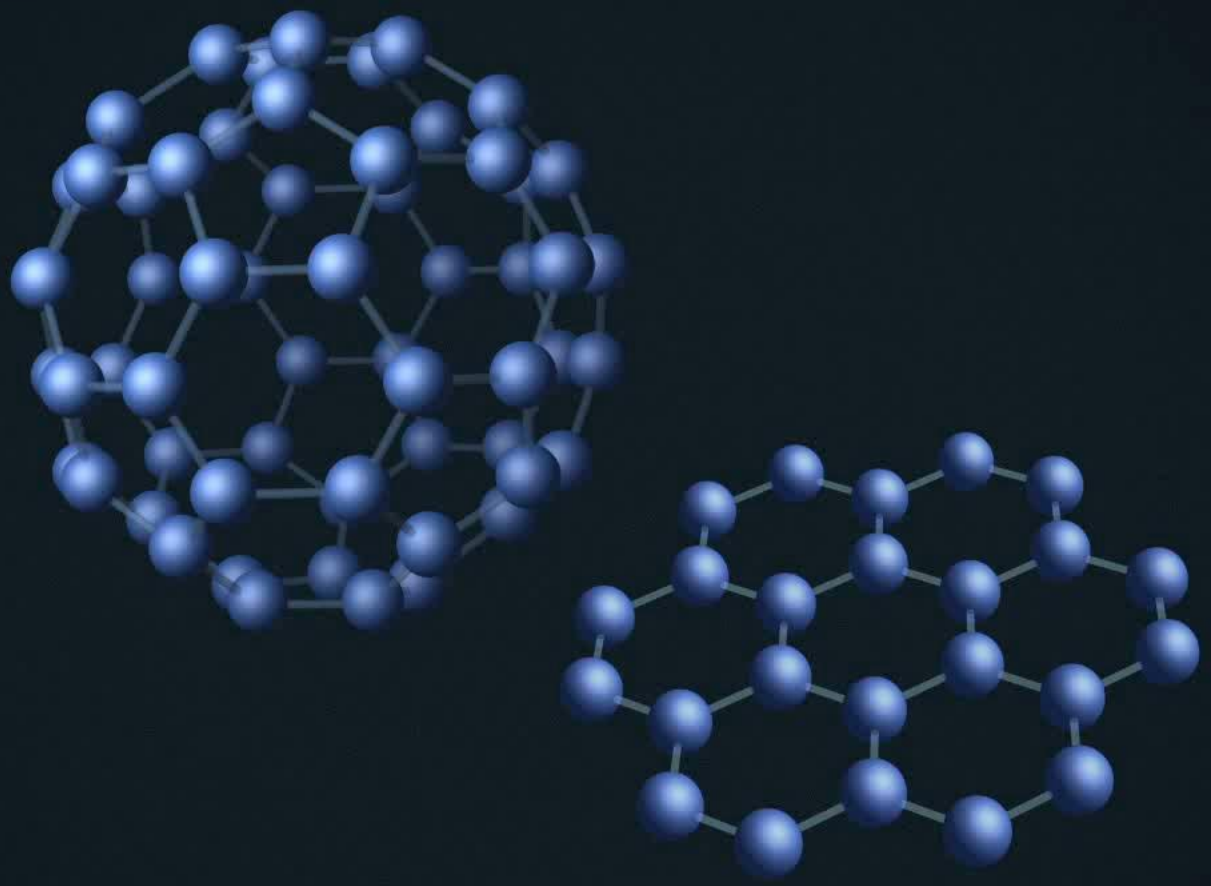
CARBON FORMS?





C60

LAB



NanoSpace

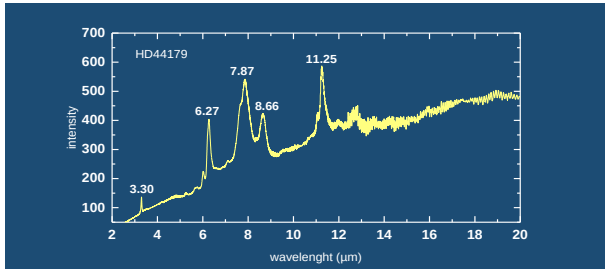
Multidisciplinary research at the IAC

- Crossing the boundaries between Astronomy, Chemistry and Physics
- Nanocarbon structures in circumstellar environments

Laboratory experiments
IACLab + Téc Lab
StarDust (ICMM)

Observations
JWST, SOFIA, IRAM, Yebes
Garcia-Hdez, Manchado
Gómez-Muñoz + Huertas-Roldán

Quantum chemistry (DFT)
Barzaga (Kerkeni)
Sadjadi (HK)/Rojas (ULL)



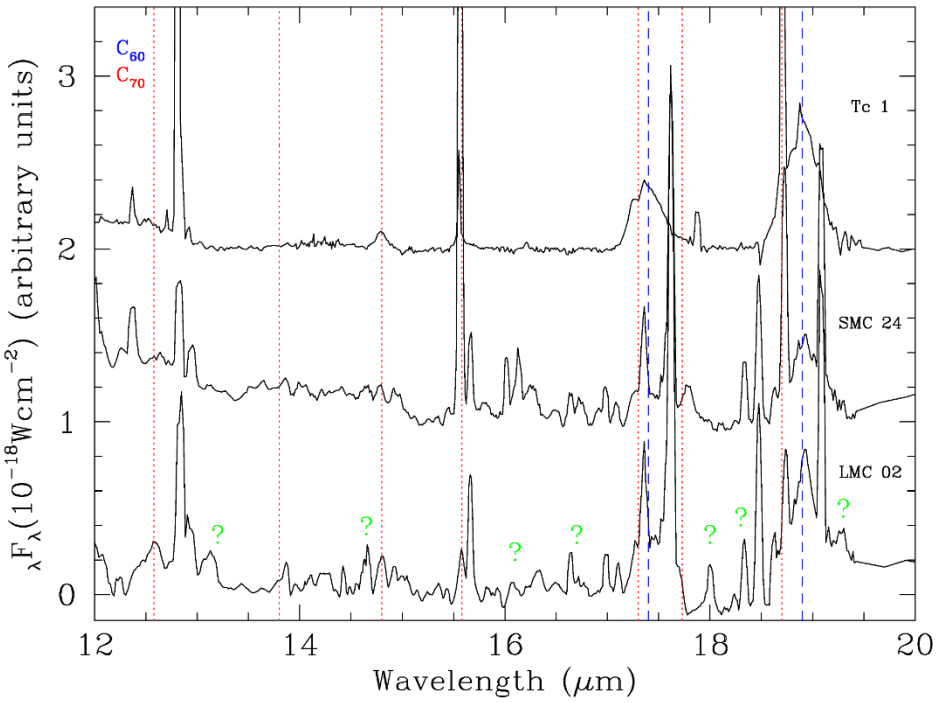
Synthetic chemistry
ACR Lab
(Cataldo)



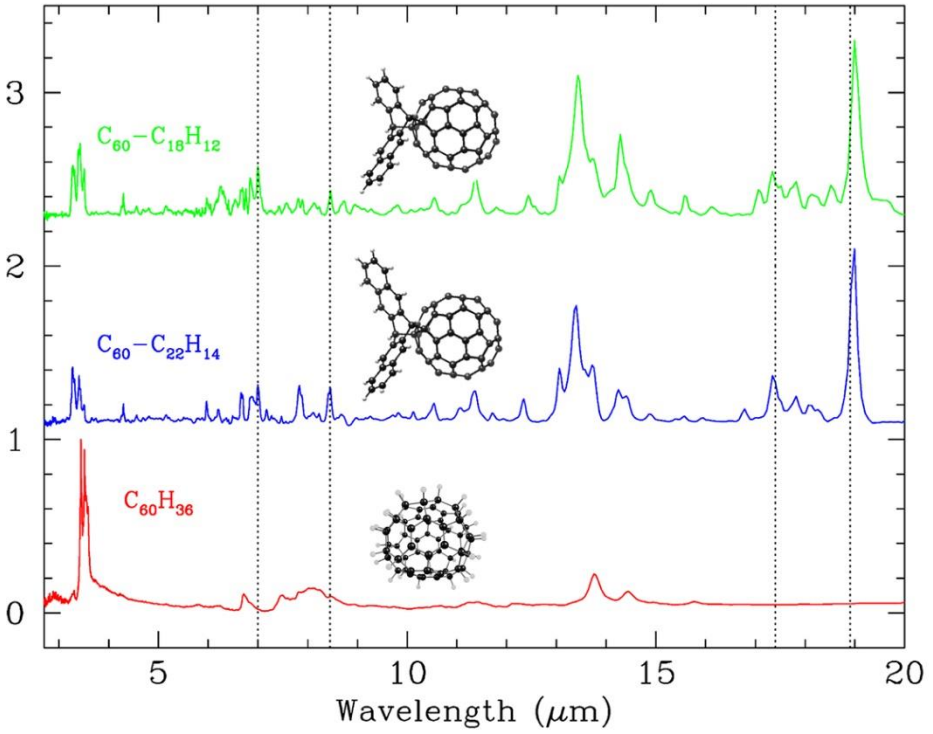
NanoSpace

The JWST potential

Confirmation of IR emission no previously detected (tentative with *Spitzer*)



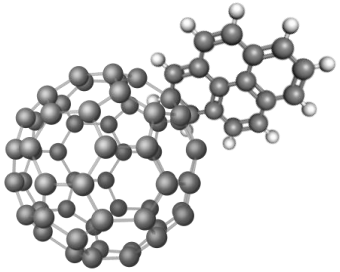
Many fullerene derivatives studied in the lab and theoretically display IR emission in JWST spectral range

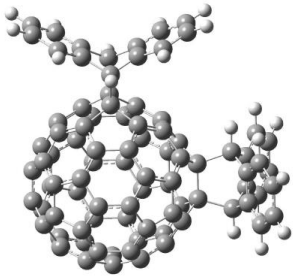


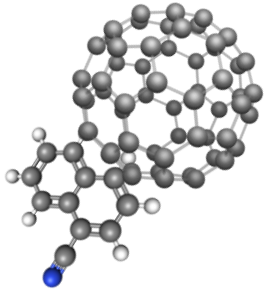
NanoSpace

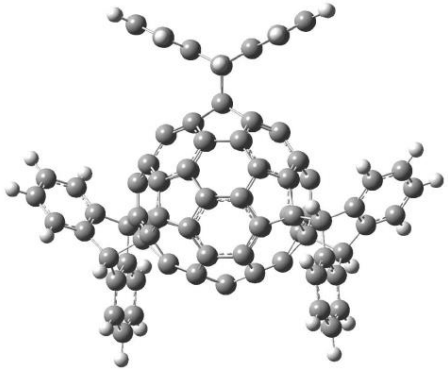
Identification of IR carriers

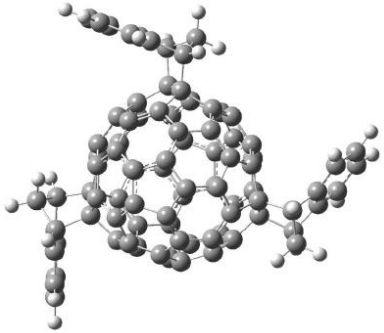
Modelling of very diverse molecules at good precision remains prohibitive

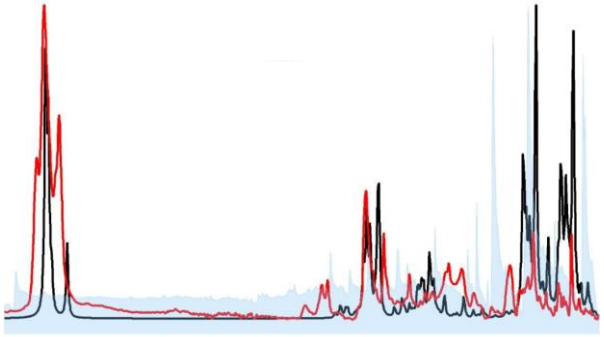












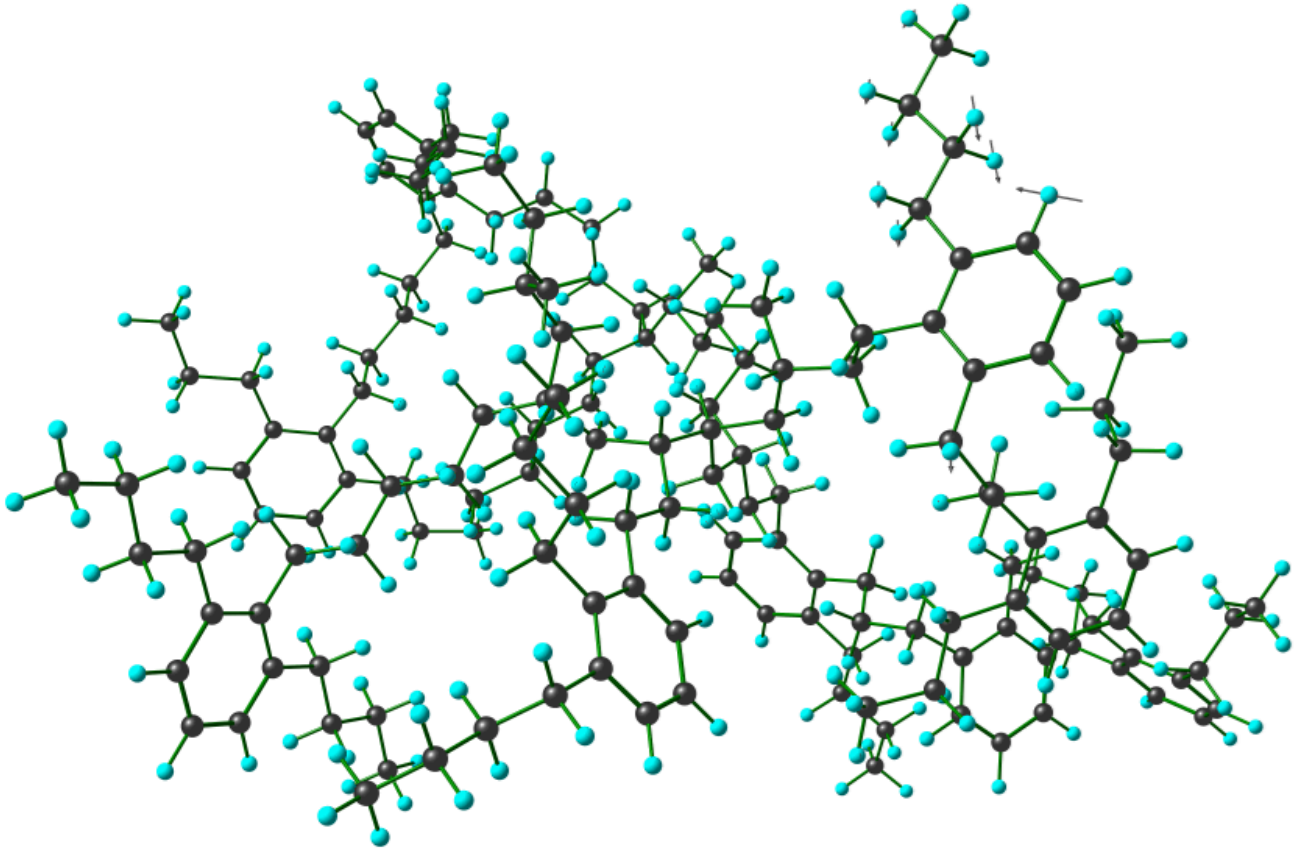
Time consuming

Lack of laboratory data

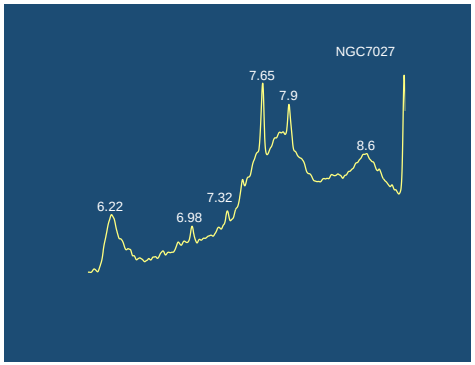
NanoSpace

Identification of IR carriers

Modelling of very large HAC-like molecules remains elusive



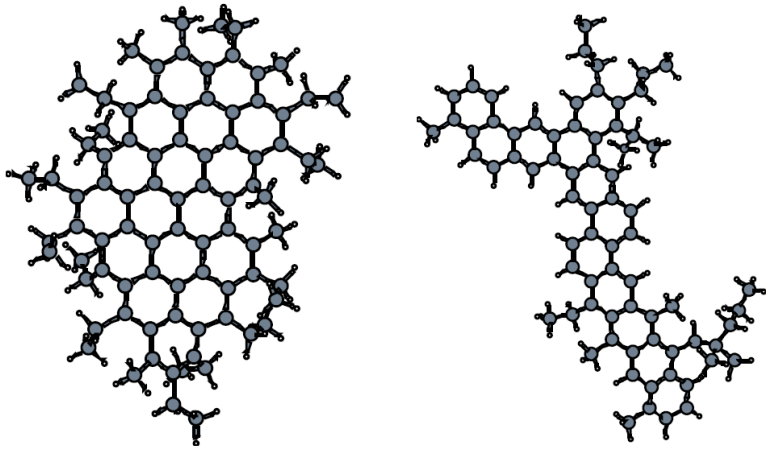
$C_{155}H_{240}$
(8.1 µm vib. mode)



Geometry for $C_{155}H_{240}$
30 CPUs , 20 days

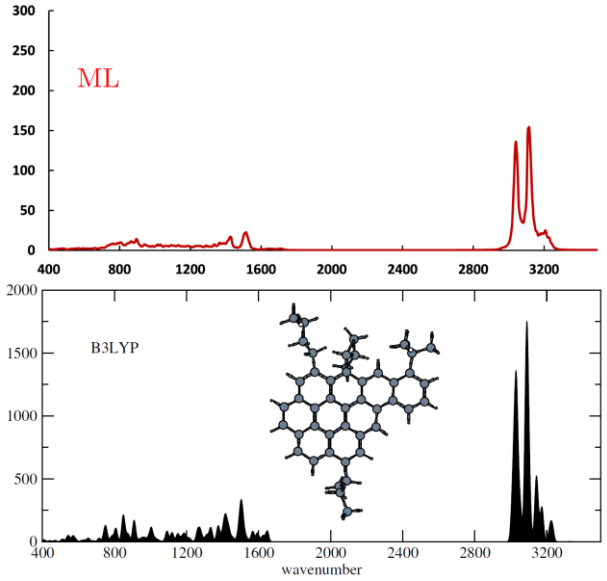
Towards carriers identification using ML

Stochastic generation of HAC-like structures (using ≠ descriptors)



NN approach predicts IR spectra from topology

Test calculations are promising for a single HAC-like structure



PCCP

PAPER

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Cite this: *Phys. Chem. Chem. Phys.*, 2017, **19**, 9934

A stochastic method for asphaltene structure formulation from experimental data: avoidance of implausible structures†

Jennifer De León, * Ana M. Velásquez and Bibian A. Hoyos

THE JOURNAL OF PHYSICAL CHEMISTRY A

pubs.acs.org/JPCA

Article

Prediction of the Infrared Absorbance Intensities and Frequencies of Hydrocarbons: A Message Passing Neural Network Approach

Maliheh Shaban Tameh, Veaceslav Coropceanu, Thomas A. R. Purcell,* and Jean-Luc Brédas*

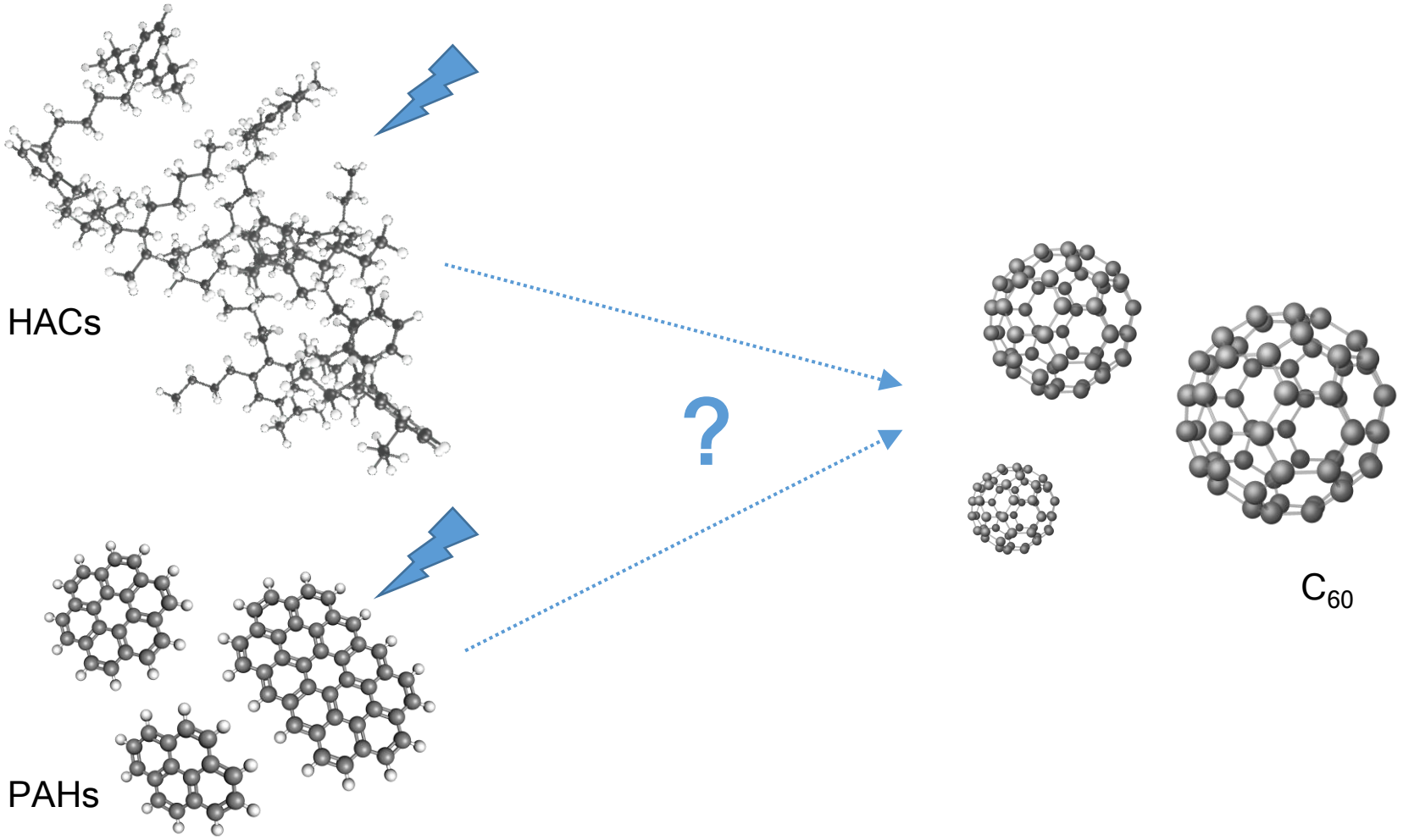
Cite This: *J. Phys. Chem. A* 2024, 128, 9695−9706

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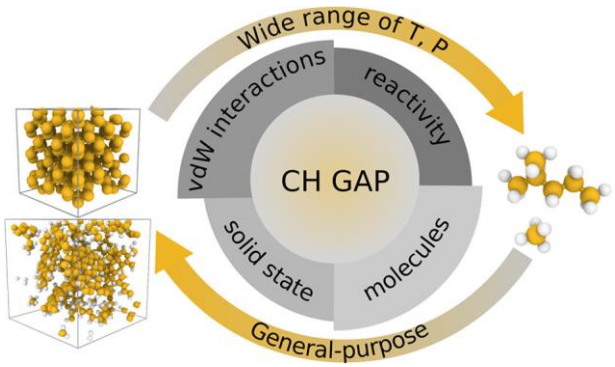
NanoSpace

Formation pathways of C_{60} species

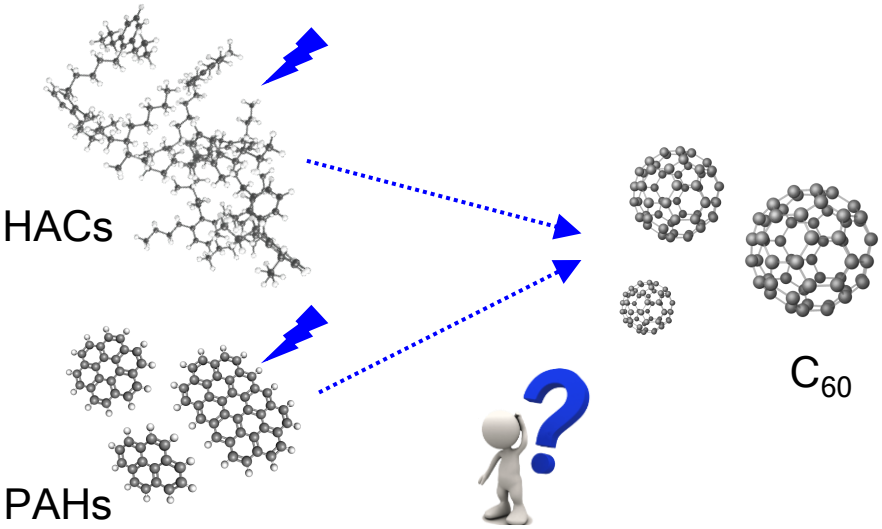
Processing/destruction (UV/high-energy radiation)

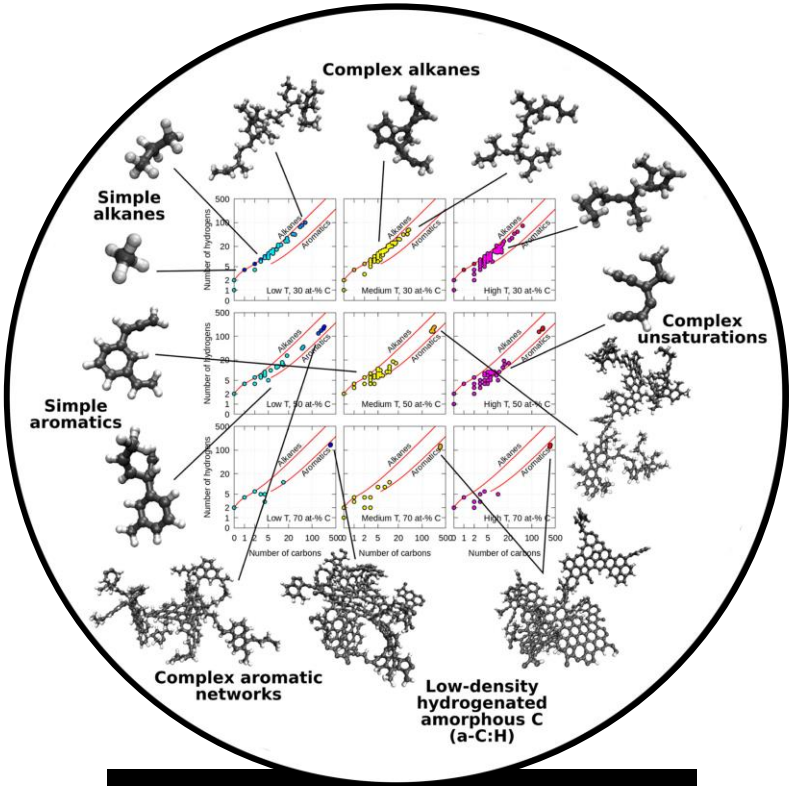


Understanding C_{60} formation via ML



Supervised learning





C-H potentials ready!

Ibragimova et al. 2025, Chem.Matt.



Motivation and overview

Artificial intelligence (AI) and machine learning (ML) have suddenly emerged as game-changing tools across diverse scientific disciplines. This includes astronomy -including observational astronomy, laboratory astrophysics and astrobiology- and chemistry -where machine learning interatomic potentials are already solidly established tools for atomistic modeling of materials and molecules. At the intersection between chemistry and astronomy, astrochemistry is posed to similarly benefit from the opportunities for accelerated scientific discovery enabled by AI. The **COST NanoSpace AI in Astrochemistry Training School 2025** aims to furnish our community with the necessary background to get started to utilize these tools, by bringing together world-renowned experts to Aalto University in Southern Finland. The School will provide **COST NanoSpace** action participants and young researchers with specialized knowledge and address the urgent need for training on AI tools in astrochemistry.

Program

The School will provide a starting point for astrochemistry researchers interested in adopting AI tools for their research. We will cover the basics as well as showcase various examples of how AI has been successfully used to tackle research problems in chemistry and astrochemistry.

Tuesday 5 August		Wednesday 6 August		Thursday 7 August		Friday 8 August	
Topic	**Trainer**	**Topic**	**Trainer**	**Topic**	**Trainer**	**Topic**	**Trainer**
Registration		Gaussian Processes and Regressors	Mads-Peter V. Christiansen	ML for Radio Interferometry	Ryan Loomis	Interpretable ML Techniques for Astrochemistry	Johannes Heyl
NanoSpace and AI in Astrochemistry TS Overview	Aníbal García-Hernández & Edward Goldwyn						
Fundamentals of ML	Miguel Caro	ML for Interatomic Potentials	Rina Ibragimova	ML Binding Energies of Astrochemical Molecules	Johannes Heyl	Exercise Session: ML for Interatomic Potentials	Rina Ibragimova
Basics of Neural Networks	Xabier Pérez Couto	Intelligent Molecular Structure Search Algorithms	Isabelle Braems	Neural Networks for Astrochemistry	Lorenzo Branca	Exercise Session: Bayesian Optimization with Gaussian Processes	Mads-Peter V. Christiansen
Exercise Session: Neural Networks I	Xabier Pérez Couto			Exercise Session: ML in Astrochemistry I	Lorenzo Branca		
Exercise Session: Neural Networks II	Xabier Pérez Couto	Atomistic Modelling for Radiation Damage in Space	Andrea Sand	Exercise Session: ML in Astrochemistry II	Lorenzo Branca	Exercise Session (continuation)	Mads-Peter V. Christiansen
Poster pitches		ML for Chemical Intuition	Brett McGuire	Excursion to Suomenlinna		Conclussions & goodbye	

NanoSpace

General

Lectures

Exercises

Posters

Social

TS Trainers



Xabier Pérez Couto



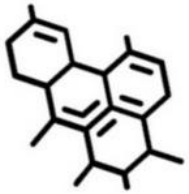
Lorenzo Branca

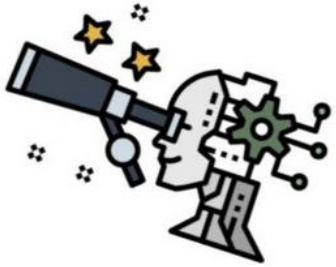


Isabelle Braems



Andrea Sand







Ryan Loomis



M-P Christiansen



Johannes Heyl

TS Organizers



Aníbal García



Miguel Caro



Rina Ibragimova



Brett McGuire



Dora Javor

Schedule and reminders

General schedule



9 to 18 hr every day

Coffee/Tea breaks



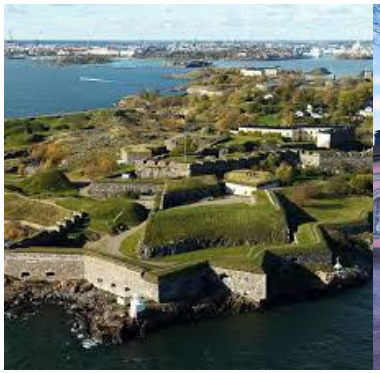
~10:30 and 15:30

Lunch break



12:30 to 14:00

Suomenlinna Excursion & Social Dinner

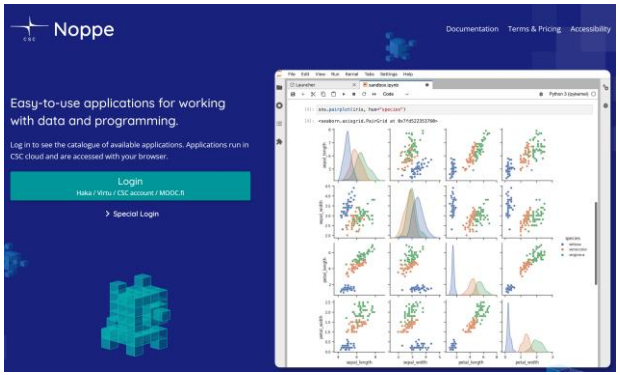




Thu 7th ~16:30 hr

Thu 7th 19:00 hr

Hands-on sessions



CSC Noppe

Att. lists



Sign!

Training School video filming

Different TS videos

Edward Goldwyn





Collaborate with Ed and NanoSpace

NanoSpace

The video plan

For the scientists who missed the TS; not public dissemination

1. Record Four Full Lectures
   - **Miguel Caro** - *Fundamentals of ML*
   - **Xabier Pérez Couto** - *Basics of Neural Networks*
   - **Isabelle Braems** - *Intelligent Crystal & Molecular Structure Search Algorithms*
   - **Brett McGuire** - *ML for Chemical Intuition*

2. Thoughts from the Lecturers
   - 3 to 5 minute presentations
   - To be either a precis of their lecture or a more general ‘thinks’ piece about the implications of the ‘Fourth paradigm’

3. An Exercise Session, one students experience
   - We need a student volunteer for the Tuesday afternoon hands-on session
   - We will record what happens

Thanks for your attention

Q & A

Unión Europea
Fondo Europeo
de desarrollo Regional
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Canarias
avanza
con Europa

Gobierno de Canarias
Consejería de Economía,
Conocimiento y Empleo

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Acknowledgements

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• COST (European Cooperation in Science & Technology) is a funding agency for research and innovation networks. Our Actions help connect research initiatives across Europe and enable scientists to grow their ideas by sharing them with their peers. This boosts their research, career and innovation.

• www.cost.eu

• https://www.cost.eu/actions/CA21126/

• https://research.iac.es/proyecto/nanospace/