NanoSpace

NanoSpace 2nd Joint Scientific Meeting & MC Meeting
Book of Abstracts

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BAU, Istanbul, Turkey
April 16 — 19, 2024

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COST Action CA21126
Carbon molecular nanostructures in space
(NanoSpace)

NanoSpace 2nd Joint Scientific Meeting 2024 & MC Meeting
April 16 — 19, 2024
BAU, Istanbul, Turkey

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Eftal Gezer
Dogan Erbahar
Domingo Anibal García Hernández

Foreword

We are pleased to welcome you to the "**2nd COST NanoSpace Joint Scientific Meeting**" taking place at Bahcesehir University, Istanbul, Turkey from 16th to 18th April 2024 (plus a half-day Management Committee meeting on 19th April 2024). The meeting will increase the interaction and collaboration among the diversity of disciplines and researchers of the Action. Special working group (WG) sessions as well as NanoSpace Database session will be part of the scientific program.

The main scope of the meeting is to increase the interactions and collaborations between the diverse disciplines (laboratory astrophysics, theoretical chemistry and physics, astronomy, among others) and researchers (especially from ITC and young researchers) present in NanoSpace towards a common language and understanding of the Action's challenge. Another scope was to finalise the internal preliminary roadmap reports for each working group, while increasing the number of participants (and interactions) to WG3 ("Role and Importance of nC in Non-Terrestrial Environments") and WG4 ("Impact, Inclusiveness and Outreach").

During the three scientific meeting days, we had an Introductory Chair talk, 7 invited Key Action Talks (lectures), 27 oral contributions, and 14 posters separated into several working group sessions, as well as database and discussions sessions.

This 2nd Joint Scientific Meeting was an excellent continuation point to share the latest research results as well as to discuss new developments and challenges in the diverse research fields; all of them related to the NanoSpace scope. This was a unique opportunity for all participants to exchange ideas, learn from each other, and find new inspirations for our research. For the ITC researchers and young researchers, in particular, it was a great opportunity for networking with other European and more senior researchers, respectively.

The 2nd COST NanoSpace Joint Scientific Meeting clearly was a step forward in our understanding of the physics and chemistry of cosmic carbon nanomaterials and their relevance in non-terrestrial environments. In addition, the preliminary Roadmap was finalized and it will be submitted to the European Physical Journal D (EPJD) during May 2024. Also, by the time of the meeting the number of participants to WG3 and WG4 has increased a factor of ~2-3.

We warmly welcome all of you to this second NanoSpace meeting in Istanbul. We hope that you will enjoy the programme, strengthening existing collaborations as well as establishing new ones.

Dr. Domingo Anibal García Hernández, Action chair

Local Organizing Committee:
Prof. Dogan Erbahar
Prof. Lutfi Arda
Eftal Gezer, BSc
Dilara Ickecan, MSc

Local Organizing Committee

Prof. Dogan Erbahar
Dogus University, Turkey

Prof. Lutfi Arda
Bahcesehir University, Turkey

Eftal Gezer, BSc
Gebze Technical University, Turkey

Dilara Ickecan, MSc
Marmara University, Turkey

Scientific Committee

Dr. Domingo Anibal García Hernández
Instituto de Astrofísica de Canarias, Spain

Prof. Eleanor Campbell
University of Edinburgh, Scotland (UK)

Dr. Chris Ewels
CNRS – Institut des Materiaux Jean Rouxell, France

Dr. Polona Umek
Jozef Stefan Institute, Slovenia

Prof. Dogan Erbahar
Dogus University, Turkey

Dr. Alicja Domaracka
CNRS – CIMAP, France

Dr. Cornelia Jäger
MPIA, Germany

Program

⛹ Scientific program

🗓 16 April 2024

Time	Title/Event	Presenter
8:00-9:00	Registration	
9:00-9:30	NanoSpace overview: where we are and where we go	Aníbal García-Hernández
	WG1 "The cosmic inventory of nC" (Session 1)	*Chair:* **Dogan Erbahar**
9:30-10:00	Complex organics in space: a changing view of the cosmos	Sun Kwok
10:00-10:30	Future directions in cosmic fullerenes	Jan Cami
10:30-11:00	*Coffee break and poster viewing*	
11:00-11:20	Mid-infrared spectroscopy of cyano-PAH cations for astrochemical consideration	Tom Douglas-Walker
11:20-11:40	Hydrogenated amorphous carbon grains as possible carriers of unexplained spectral phenomena in evolved stars	Arturo Manchado
11:40-12:00	Determination of optical properties of amorphous carbon from the measured reflection electron energy loss spectroscopy spectra	Karoly Tőkési
12:00-12:20	Asphaltenes as model compounds of the possible carriers of the UIBs/AIBs detected in various astrophysical objects	Franco Cataldo
12:30-14:00	*Lunch*	
	WG2 "Processing, reactivity and relaxation pathways of nC" (Session 2)	*Chair:* **Chris Ewels**
14:00-14:30	Tracing the origin and evolution of cosmic PAHs: molecular analysis of dust analogs and meteorites	Hassan Sabbah
14:30-14:50	Effect of swift ion irradiation on pyrene	Anna Bychkova
14:50-15:10	Photoprotonation of a carbon atom of an aromatic ring	Nađa Došlić
15:10-15:30	Stabilities of highly reactive nanocarbon ions	Henning Zettergren
15:30-16:00	*Coffee break and poster viewing*	
16:00-16:20	Ion irradiation of astrophysical ices: implications for formation of complex molecular species	Alicja Domaracka
16:20-16:40	Photo-processing of carbonaceous dust grains by water ice	Cornelia Jäger
16:40-17:00	Effect of gamma radiation on structure, morphology, and optical properties of GO/PVA nanocomposite	Lala Gahramanli
17:00-17:30	**Flash Poster Session** (1-2 minutes informal poster presentations & discussion)	

📅 17 April 2024

Time	Title/Event	Presenter
	WG3 "Role and Importance of nC in Non-Terrestrial Environments" (Session 1)	*Chair:* **Cornelia Jäger**
9:00-9:30	Exploring the cosmic origins of prebiotic molecules through laboratory interstellar ice experiments	Cornelia Meinert
9:30-10:00	Quantum chemical study of complex organic molecules in the interstellar medium	Boutheïna Kerkeni
10:00-10:20	Fullerenes as versatile catalysts in prebiotic reactions	Eftal Gezer
10:30-11:00	*Coffee break and poster viewing*	
11:00-11:20	Low-temperature photochemistry of sulfur-containing complex organic molecules	Marcin Gronowski
11:20-11:40	Electronic and optical properties of molecules calculated within DFT based schemes: from PAHs to nucleobases	Giancarlo Cappellini
	WG1 "The cosmic inventory of nC" (Session 2)	*Chair:* **Cornelia Jäger**
11:40-12:10	Unveiling the photochemical evolution of carbonaceous molecules: experimental and theoretical studies	Alessandra Candian
12:10-12:30	Fullerene derivatives from single metal atoms to molecules: A quantum chemistry perspective	Ransel Barzaga
12:30-14:00	*Lunch*	
	WG1 "The cosmic inventory of nC" (Session 2)	*Chair:* **Polona Umek**
14:00-14:20	Almost complete classification of carbon molecules based on their conductivity	Irene Sciriha
14:20-14:40	Topological data analysis of fullerene graph spectra	Tomislav Došlić
	WG4 "Impact, Inclusiveness and Outreach" (Session 1)	*Chair:* **Polona Umek**
14:40-15:00	Cosmic nanocarbon inventory database proposal: A sustainable, open-access and open-source Science 4.0 platform	Eftal Gezer
15:00-15:20	Storing and sharing computational data through comprehensive databases	Ana Martín Somer
15:30-16:00	*Coffee break and poster viewing*	
16:00-17:00	**Database Discussion Session**	
19:00	***Conference Dinner***	

📅 18 April 2024

Time	Title/Event	Presenter
	WG2 "Processing, reactivity and relaxation pathways of nC" (Session 2)	*Chair:* **Alicja Domaracka**
9:00-9:30	Theoretical modelling of nanocarbon materials using machine learning approaches	Rina Ibragimova
9:30-9:50	Atomic scale investigations on nanodiamond materials via TEM	Raúl Arenal
9:50-10:10	Nanocarbons and how to compute your way out of experimental problems	Manuel Melle Franco

10:10-10:30	A theoretical study on the mechanisms of formation of primal carbon clusters and nanoparticles in space	Stefan Kolev
10:30-11:00	*Coffee break and poster viewing*	
	WG4 "Impact, Inclusiveness and Outreach" (Session 2)	*Chair:* **Flavia Dell'Agli**
11:00-11:20	Chemical functionalization of multilayers fullerenes (carbon nano-onions) for biomedical applications	Silvia Giordani
11:20-11:40	Emergent atomic environments in twisted bilayer graphene and their use in the prediction of the vibrational properties	Dogan Erbahar
11:40-12:00	Using quantum computer assistance to scale up quantum correlation measures for nC	Barış Malcıoğlu
12:00-12:20	Investigating devices that measure nanocarbon molecular structures in space	Musa Akbulut
12:30-14:00	*Lunch*	
14:00-14:20	Metal-semiconductor transition investigation of nanocrystalline silicon carbide under irradiation in space technology	Elchin Huseynov
14:20-15:30	**Panel Discussion Show Session**	*Moderator:* **Jan Cami**
15:30-16:00	*Coffee break and poster viewing*	
16:00-16:30	**Final Joint Discussion**	*Moderator:* **Eleanor Campbell**

⠿ Poster presentations

#	Title	Presenter
1	Enhancing the thermal stability of TiO2-B nanoribbons	Polona Umek
2	Action spectroscopy of CN containing PAH cations	Ewen Campbell
3	Machine learning methods for DFT simulations of nanostructures	Ioannis Remediakis
4	Diameter of nanotori	Vesna Andova
5	Theoretical and EIS investigation of the formation of oxygen on the hematite surface	Veton Haziri
6	Structure and spectroscopy of molecules of astrochemical interest and their aggregates with water	Ana Niedojadlo
7	Using concepts of computer games development to create a data visualisation engine	Simon Scarle
8	STM observation and characterisation of azafullerene radicals	Yuri Tanuma
9	STM studies of C60 cage shrinking on Cu(111)	Eleanor Campbell
10	EiBI gravity-modified solar GES structure	Souvik Das
11	Balancing error and scaling in quantum computer with machine learning	Kaan Yurtseven & Özgür Nazlı
12	Shaping tomorrow: breaking bias in childhood education	Flavia Dell'Agli
13	Influence of thermal annealing on the physical properties of GO composite materials	Lala Gahramanli
14	Age-mass ratio and evolution of the herbig AeBe stars	Sabahaddin Alishov

⚙ Management Committee (MC) meeting

Only MC members and individuals with Action leadership positions and/or invited are attending the MC meeting.

📅 19 April 2024

Time	Session/Event	Moderator
9:00-10:30	**MC Meeting (Session 1)**	**Aníbal García-Hernández**

1. Welcome to participants, verification of the quorum and adoption of agenda
2. Information to the MC
   a. Recap of the minutes of the last meeting, e-votes and matters arising since the last meeting
   b. Core Group: report from the Core Group, including delegated decisions
   c. Action Membership: New Specific Organisations and COST Members represented in the MC
   d. Action Participation: WG membership and applications, New MC Members/Observers

   and provisional substitution.

   e. Budget status: summary from the Grant Holder
   f. Update from the COST Association (if representative is present)

10:30-11:00	*Coffee break*	
11:00-14:00	**MC Meeting (Session 2)**	**Aníbal García-Hernández**

3. Follow up and discussion on the
   a. Action management: structure, leadership positions and other supporting roles.

   Mandates to the Core Group (if applicable)

   b. Implementation of the COST Excellence and Inclusiveness Policy
   c. Grant Awarding by the Action
   d. Progress of each working group
   e. Science Communication Plan
   f. Progress on MoU Objectives, WG tasks, deliverables, and Goals for the current GP.
4. Planning
   a. Revision of Work and Budget Plan of the current GP (if applicable)
   b. Draft plans for the following GP(s).
   c. Upcoming activities
5. Monitoring and Reporting to the COST Association
6. AOB
7. Summary of MC decisions
8. Closing

Contents

Poster Presentations   **40**

Invited Lectures

NanoSpace overview: where we are and where we go

D. A. García-Hernández[1,2,*]

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It is now ~1,5 years that the COST Action NanoSpace ("Carbon molecular nanostructures in space"; CA21126) is successfully running. I will present a short overview of the Action with a particular attention on where we are and where we go. This will include the main motivation, scientific challenges, objectives, and deliverables together with the most recent updates. Examples of the diverse networking activities already carried out (or planned) in order to increase the interactions and collaborations between the diverse disciplines (laboratory astrophysics, theoretical chemistry and physics, astronomy, among others) and researchers (especially from ITC and young researchers) present in NanoSpace will be provided.

Complex Organics in Space: a changing view of the cosmos

Sun Kwok[1,2]

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Planetary explorations have revealed that complex organics are widely present in the Solar System. Astronomical infrared spectroscopic observations have discovered that complex organics are synthesized in large quantities in planetary nebulae and distributed throughout the Galaxy. Signatures of organics are found in distant galaxies, as early as 1.5 billion years after the Big Bang. Several unsolved spectral phenomena such as diffuse interstellar bands, extended red emissions, 220 nm feature, and unidentified infrared emission bands are likely to originate from organics. In this paper, we discuss the possible chemical structures of the carriers of these phenomena, and how these organics are synthesized abiotically in the Universe. The implications of possible stellar organics in primordial Earth are also discussed.

Future Directions in Cosmic Fullerenes

J. Cami[1,2,3]

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[2] *Department of Physics & Astronomy, Western University, London, Canada*
[*] *jcami@uwo.ca*

Fullerenes have been detected in a variety of astrophysical environments – from the circumstellar carbon-rich surroundings of evolved stars to diffuse clouds, interstellar reflection nebulae and young stellar objects. Most detections involve emission through the infrared vibrational transitions of the neutral species C_{60}. At the same time, the cation $C_{60}^{+¿¿}$ has been identified as the carrier of 2 strong and 3 weaker diffuse interstellar bands (DIBs). Cosmic fullerenes have thus been firmly identified, and offer a unique opportunity to study the formation, evolution, excitation and detailed molecular physics of large aromatic species in space.

In this talk, I will give an overview of the environments where we have detected fullerenes. I will summarize the key observational properties as well as what we have learned from these detections. I will highlight some of the remaining issues we face in understanding these observations, and how laboratory experiments, theoretical calculations and future observatons will help coming up with a coherent picture for the life cycle of fullerenes and related carbonaceous species in space.

Tracing the Origin and Evolution of Cosmic PAHs: Molecular Analysis of Dust Analogs and meteorites

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Large carbonaceous molecules, such as polycyclic aromatic hydrocarbons (PAHs), are abundant in astrophysical environments, and play a significant role in the physics and chemistry of regions where stars and planets form. Investigating the formation and evolution of specific molecules within these families, notably in the hot and dense envelopes of evolved stars, has ignited numerous research endeavors to synthesize cosmic dust analogs using diverse techniques. Additionally, analyzing primitive extraterrestrial materials, such as carbonaceous chondrites and samples returned from asteroid missions, offers promising insights into the origin and evolution of these molecules.

The experimental setup, AROMA [1] (Astrochemistry Research of Organics with Molecular Analyzer), has unique capabilities for probing PAHs, carbon clusters, and fullerenes in both primitive extraterrestrial matter and cosmic dust analogs. The setup consists of a laser desorption ionization source and a segmented linear quadrupole ion trap connected to an orthogonal time-of-flight mass spectrometer. Notable results obtained so far include analyses of cosmic dust analogs generated by the Stardust machine [2] and through in-flame combustion soot [3], as well as the detection of fullerenes in the Almahata Sitta meteorite [4].

References

[1] H. Sabbah et al., *The Astrophysical Journal* 843, 34 (2017)

[2] L. Martínez et al., 2019, *Nature Astronomy* 4, 97 (2019)

[3] H. Sabbah et al. *Proceedings of the Combustion Institute*, 38, 1241 (2021)

[4] H. Sabbah et al., *The Astrophysical Journal* 931, 91 (2022)

Exploring the Cosmic Origins of Prebiotic Molecules through Laboratory Interstellar Ice Experiments

C. Meinert[1*], A. Turner[2], R. Kaiser[2], G. Danger[3], L. d'Hendecourt[3]

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The quest to understand the origins of life takes us on a cosmic journey, where intricate chemical reactions in interstellar environments may hold the key to unlocking the mysteries of our existence (Fig 1). In this talk, I'll highlight our most recent laboratory interstellar ice experiments, shedding light on the formation of prebiotic molecules, including sugars [1], as well as organic sulfurous and phosphorous compounds [2].

Through laboratory experiments and quantum calculations, we have uncovered the chemical pathways through which these essential molecules emerge in molecular cloud ices. Moreover, our recent investigations have extended beyond the cold depths of interstellar space, delving into the evolution of these ices within our solar system. By subjecting interstellar ice analogs to energetic processing and aqueous alteration, we have elucidated the complex interplay between cosmic radiation, thermal alteration, and chemical reactions, shaping the molecular complexity of these icy reservoirs [3] and their surface colors [4].

Our findings not only illustrate how complex organic molecules can form under very cold conditions but also pave the way for a deeper understanding of the vast network of chemical evolution that permeates the universe. So, please join me as we embark on a journey to unravel the cosmic origins of prebiotic molecules, bridging the divide between the distant cosmos and the intimate chemistry of life on Earth.
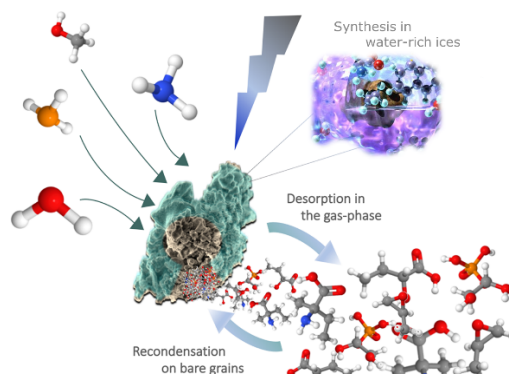
Figure 1: Energetic processing reproduces the evolution of interstellar ices observed in molecular clouds.

Acknowledgements

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[4] C. Zhang, et al., *Science Advances* **9**, eadg6936 (2023)

Quantum Chemical Study of Complex Organic Molecules in the Interstellar Medium

B. Kerkeni[1]

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More than 200 species have been detected in the interstellar medium (ISM), among them many molecules, radicals and ions, containing the −C≡N functional group. To date, PrCN is one of the most complex molecules found in the interstellar medium. Furthermore, it is the only one observed species to share the branched atomic backbone of amino acids, some of the building blocks of life. Radical-radical chemical reactions in gas phase and on an ice model are examined in detail using density functional theory M062X/6-311++g(d,p) and *ab initio* methods CCSD(T)-F12//MP2. The reaction mechanism involves the following radicals association: CH3CHCH3+CN, CH3+CH3CHCN for iso-PrCN and CH3CH2+CH2CN, CH3 +CH2 CH2 CN, CN+CH3 CH2 CH2 for n-PrCN formation. All reaction paths are exoergic and barrier-less in the gas phase and on the ice-model, suggesting that the formation of iso-PrCN and n-PrCN is efficient on the water-ice model adopted

Another molecule: acetaldehyde (CH₃CHO) is ubiquitous in interstellar space and is important for astrochemistry as it can contribute to the formation of amino acids through reaction with nitrogen containing chemical species. Quantum chemical and reaction kinetics studies are reported for acetaldehyde formation from the chemical reaction of C(^{3}P) with a methanol molecule adsorbed at the eighth position of a cubic water cluster. We present extensive quantum chemical calculations by means of CCSD(T)//wB97XD/6-311++G(2d,p) for total spin S=1 and S=0.

CH3+CH3CHCN → iso-PrCN
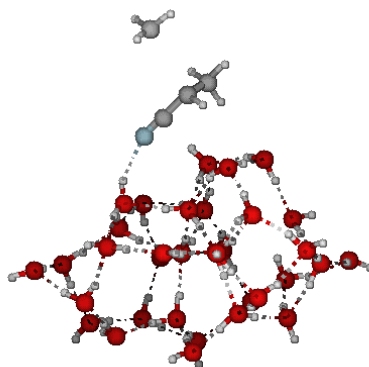
References

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Unveiling the photochemical evolution of carbonaceous molecules: experimental and theoretical studies.

A. Candian[1]

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The new stunning observations delivered by the James Webb Space Telescope are revolutionizing our view of the molecular universe, in particular when it comes to large carbon-containing species such as Polycyclic Aromatic Hydrocarbons (PAHs) and carbon cages. The infrared spectra show a treasure of spectroscopic features that change in response to the physical conditions in the astronomical object and thus speak of active photochemistry shaping the population of carbonaceous molecule [1,2].

The synergies between experiments, quantum chemistry calculations and modelling are fundamental to get insight on the behavior of molecules in the interstellar medium and interpret the observations. In this talk I will present the latest efforts to constrain how the molecular properties of PAHs (eg. size, shape) influence their photochemistry.

References
[1] R. Chown and PDRs4All team, *Astronomy and Astrophysics*, forthcoming (2023)
[2] S. Pasquini, and PDRs4All team, *Astronomy and Astrophysics*, accepted (2024)

Theoretical modelling of nanocarbon materials using machine learning approaches

R. Ibragimova[*1], M. A. Caro[1]

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Machine learning (ML) techniques have revolutionized the fields of materials science and physics by providing fast and accurate solutions to complex problems. In this talk, we will explore the exciting possibilities that ML presents for constructing interatomic force fields or interatomic potentials (MLPs) for modeling various phenomena in materials science and solid-state physics.

Specifically, I will focus on the Gaussian Approximation Potential (GAP) framework [1], which has become a popular method for training MLPs and accurately predicting atomic forces and energies of materials. I will present recent results on training general-purpose reactive MLPs for carbon and hydrogen (CH), carbon and oxygen (CO) systems [2-3], discussing their relevance to atomistic modeling of nanocarbon synthesis and its characterization for astrochemistry.
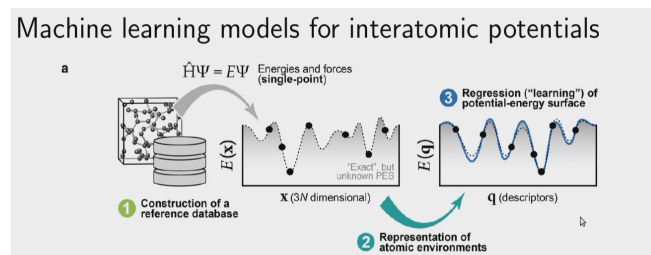
Figure 1: Schematics of MLP training procedure [4]

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Oral Presentations

Mid-infrared spectroscopy of cyano-PAH cations for astrochemical consideration

T. E. Douglas-Walker[1], F. C. Daly[1], A. Zheng[1], J. Palotás[1] and E. K. Campbell[*1]

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Polycyclic aromatic hydrocarbons (PAHs) have been proposed as carriers of the unidentified infrared bands (UIBs), a series of IR emission lines detected from various regions of the interstellar medium [1]. Cyano-group containing aromatic structures such as benzonitrile [2], cyanonaphthalene [3] and cyanoindene [4], have recently been detected in interstellar clouds based on their laboratory rotational spectrum by radio astronomy. However, there is a paucity of laboratory IR measurements of gas-phase cyano-PAH cations for comparison to observational data. Here we present the low temperature gas-phase vibrational spectra of a set of ionized cyano-group containing PAHs in the mid-infrared region [5]. Experimentally, the ions are cooled at 4 K in a cryogenic ion trapping apparatus, tagged with He atoms and probed with tunable radiation.
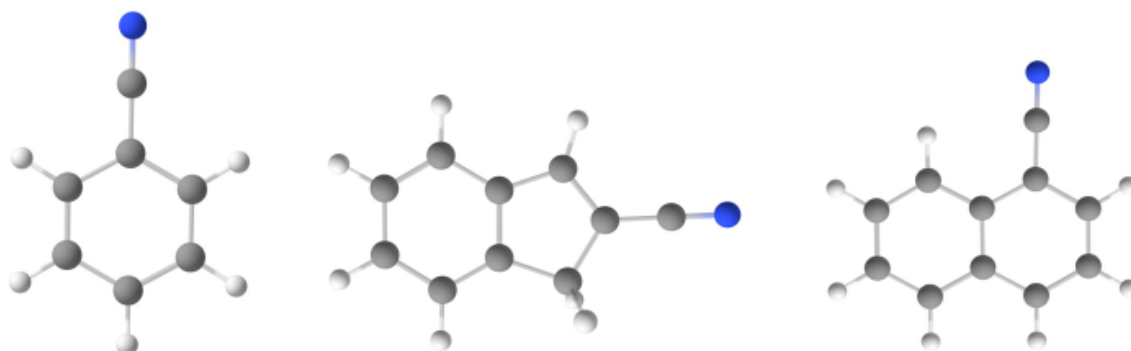
Figure 1: Optimized geometry of a) benzonitrile, b) cyanoindene and c) cyanonaphthalene cations

Acknowledgements

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[1] A. Léger and J. L. Puget, *Astron. Astrophys.*, **137**, L5 —L8 (1984)
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Hydrogenated amorphous carbon grains as possible carriers of unexplained spectral phenomena in evolved stars

A. Manchado[1,2,3], M. A. Gómez-Muñoz[1,2], D. A. García-Hernández[1,2], R. Barzaga[1,2], T. Huertas-Roldán[1,2]

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[2]Universidad de La Laguna, La Laguna, Spain
[3]Consejo Superior de Investigaciones Científicas, Spain

The mid-infrared spectra of a particular group of evolved stars like fullerene-rich planetary nebulae (PNe) are dominated by aliphatic hydrocarbon-rich dust, showing several broad unidentified infrared (UIR) emission features such as the 6-9 (7µm hereafter) and the 9-13-micron (12µm hereafter) plateau emission features (Fig.1), among others. In particular, the 7 and 12µm plateau emission features have been suggested to emerge from hydrogenated amorphous carbon (HAC) dust grains or similar mixed aliphatic-aromatic hydrocarbon nanoparticles (HAC-like). Similarly, HAC-like grains, and other carbonaceous materials, have been also suggested to be responsible for some ultraviolet (UV) absorption features like the so-called UV-bump and the far-UV rise. The laboratory optical constants of specific (in terms of structure/composition) HAC-like dust grains have been recently used in conjunction with radiative transfer codes, demonstrating for the first time that HAC-like dust grains convincingly reproduce the 12µm plateau emission feature observed in the prototypical fullerene-rich PN Tc 1 (and still consistent with the dust continuum and 7µm plateau emissions; Fig. 1) [1]. Interestingly, the same HAC-like grains may reproduce the far-UV rise circumstellar extinction observed towards PN Tc 1 and similar evolved stars [2]. The possible detection of HAC-like dust grains in the circumstellar envelopes of PNe is of special interest to the fullerene formation mechanism, suggesting that fullerenes around evolved stars could be formed by the processing and/or destruction of HAC-like dust [1,2]. These very recent works [1,2] strongly encourage more laboratory experiments to obtain the refractive indices (n and k) of HAC-like dust grains with several structures/compositions in order to extend this kind of modelling studies to more evolved stars and/or even other astrophysical objects.

Figure 1 – Top-panel: The C_{60} and C_{70} fullerenes sketch. Bottom-panel: Spitzer IR spectrum of the PN Tc 1 (black) compared with a photoionization model including the HAC dust grains (green). The C_{60} (blue) and C_{70} (red) emission bands and broad UIR emissions are indicated. Adapted from [1].

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Determination of optical properties of amorphous carbon from the measured reflection electron energy loss spectroscopy spectra

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In recent years a well-established analysis technique based on reflection electron energy loss spectroscopy (REELS) has been developed to obtain optical constants in a rather wide range of energy loss of electrons. The method is called reverse Monte Carlo (RMC) method. It integrates the Monte Carlo simulation of REELS spectrum and Marokv chain Monte Carlo technique for updating of the energy loss function during the circle of the simulation [1].

In this work, we present the combined experimental and theoretical investigations of optical properties of amorphous carbon based on RMC method. The REELS spectra of carbon were measured at primary electron energies of 750, 1000 and 1300 eV. The energy loss function and thereby the refractive index n and the extinction coefficient k were extracted from these REELS spectra in a wide loss energy range of 2-200 eV. The high accuracy of the obtained optical constants is justified with the ps- and f-sum rules. We found that our present optical constants of amorphous carbon fulfill the sum rules with the higher accuracy as compared with the previous published data [2]. Therefore, we highly recommend the use of the present data in a practical application.

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Asphaltenes as model compounds of the possible carriers of the UIBs/AIBs detected in various astrophysical objects

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The Unidentified Infrared bands (UIBs or UIRs) known also as Aromatic Infrared Bands (AIBs) represent a series of discrete infrared emission bands detected in numerous and different astrophysical objects [1]. The carriers of these infrared bands have not yet fully identified. The MAONs model proposes that the carriers of the UIBs could be described by an "average" chemical structure consisting of mixed aromatic-aliphatic organic nanoparticles and containing also heteroatoms such as N, S, and O [2]. The asphaltenes derived from certain heavy petroleum fractions and other natural sources are matching quite well the MAONs model [3-5]. The aliphatic/naphthenic/aromatic content can be modulated by thermal treatment or by high energy processing, increasing the aromatic content till the chemical structure of a carbon coke [3-4]. Both the starting asphaltenes and the thermally and radiation processed asphaltenes were studied with FT-IR spectroscopy [3-5]. A new molecular imaging techniques has recently been developed to the stage that the asphaltene molecules can be "seen" as individual molecular structures [6,7]. This new molecular imaging technique is based on atomic force microscopy coupled with scanning tunneling microscopy (AFM-STM) [6,7]. In this presentation, a survey of the most recent and exciting results applied to the asphaltene molecules derived from petroleum, coal, and thermal processing (and used by us as MAON models) will be reviewed.

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Effect of swift ion irradiation on pyrene

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Polycyclic Aromatic Hydrocarbons (PAHs) are believed to represent 15% of all carbon in the ISM both in gas and in solid phases [1]. When PAHs are exposed to ionizing radiation, they can be destroyed. It is therefore important to study the resistance of PAHs to ionizing radiation and to predict their lifetime in space. We report the results of an experimental study of the irradiation of the PAH molecule pyrene at 20K. The experiments were performed at the Ice Chamber for Astrophysics-Astrochemistry [2] at the Tandetron facility of ATOMKI (Debrecen, Hungary). Fig. 1 shows the decrease of the pyrene 710 cm^{-1} IR band area as a function of deposited local dose for 11 projectiles.
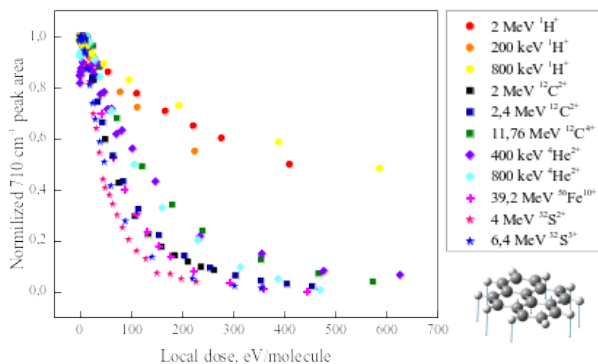
Figure 1: Normalized 710 cm^{-1} pyrene IR band as a function of local dose. Irradiations with 11.67 MeV C and 39.2 MeV Fe were performed at GANIL-IRRSUD

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Photoprotonation of a Carbon Atom of an Aromatic Ring

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Excited-state proton transfer (ESPT) reactions typically occur between a proton donor (e.g., NH or OH) and an electronegative heteroatom.[1] Sometimes, however, the proton acceptor can be a carbon atom.[2] In 2002, Wan *et al.* reported the first example of direct photoprotonation of a carbon atom of an aromatic ring via excited-state intramolecular proton transfer (ESIPT).[3] At first glance, ESPT to a carbon atom is somewhat surprising, since protonation of an aromatic carbon atom typically is a slow process in the ground state. Yet, why do some aromatic ring carbons gain basicity in the excited-state?

Excited-state antiaromaticity relief can play important roles in many light-driven proton and electron transfer reactions. Here, we report on the photo-protonation mechanism of three aminobiphenyl isomers. In all three cases, a proton formally migrates from an NH_2 group to an aromatic ring carbon atom. All three isomers*, ortho-, meta-,* and *para-*, can undergo ESPT involving water. In addition, the *meta*-isomer can undergo a photoredox reaction, involving proton-coupled electron transfer and water-splitting. We suspect that strong antiaromaticity in the aniline ring may be responsible for driving the observed reactions.
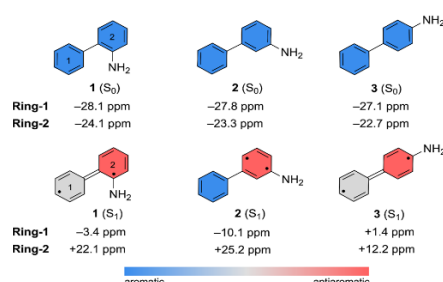
Figure 1: Computed NICS(1)zz values for the S0 and S1 state minimum geometries of 1-3

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Stabilities of highly reactive nanocarbon ions

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The cryogenic electrostatic ion beam storage ring facility DESIREE (Double ElectroStatic Ion Ring ExpEriment) at Stockholm University offers unique possibilities to study interactions with internally relaxed molecular and cluster ions and their internal cooling dynamics in new time domains and in unprecedented details. We have recently developed a technique where we store single or a few ions at a time, which we have used to study the stability of highly reactive carbonaceous molecules [1-3]. These include fullerene [1] and PAH [2] fragments where individual carbon atoms have been knocked out in collisions with helium atoms at velocities typical for gas in interstellar shocks and stellar winds, and we have shown that they may survive indefinitely in isolation. Furthermore, we have shown that the intrinsic lifetime of the smallest long-lived all carbon molecular dianion, C_7^{2-} (Fig.1), exceeds several minutes [3]. This is six orders of magnitude longer than established from earlier experiments.
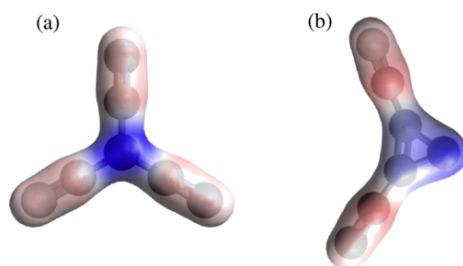
Figure 1: We have studied the stability of C_7^{2-} in new time domains and with a single ion at a time. The molecular structures shown in this figure are the two most stable C_7^{2-} isomers according to our quantum chemistry calculations and model calculations of tunneling rates [3].

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Ion irradiation of astrophysical ices: implications for formation of complex molecular species

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"What is the origin of organic matter in the universe? " is one of important question of astrophysics. Complex organic molecules have indeed been observed in space (comets, meteorites, molecular clouds). Synthesis of complex organic molecules (COMs) is possible in different astrophysical environments. On the one hand, it has been shown that COMs are formed by radiolysis of small molecules (H_2O, CO, CH_4, NH_3 etc.) on cold surfaces of icy bodies in the outer solar system or grains in the dense molecular clouds) [1]. On the other hand, molecular complexification can also take place in solar system via implantation of ions trapped in the magnetospheres of giant planets into the icy surfaces of their satellites (like e.g. C or S ejected by Io's volcanism impacting Europe) [1].

Recent experiments at the GANIL ion beam facility (Caen, France) in collaboration with A. Bouquet (PIIM, Marseille, France) have evidenced that implantation of sulfur ions in ice samples ($H_2O:C_3H_8$), in conditions relevant to Europa and other Jovian satellites contribute considerably to synthesis of complex molecular species. Refractory residue, which was formed after ion irradiation, was analyzed by means of Ultra-High Resolution Mass Spectrometry techniques, using two ionization techniques (laser desorption and electrospray). The results revel a very diverse organic matter (more than 2500 unique molecular formulas) with heavy molecules (m/z>200, up to 1200) being common, like large numbers of aliphatic and aromatic CH species (PAHs), fullerenes, as well as organosulfurs (CHS form and CHOS) [3].
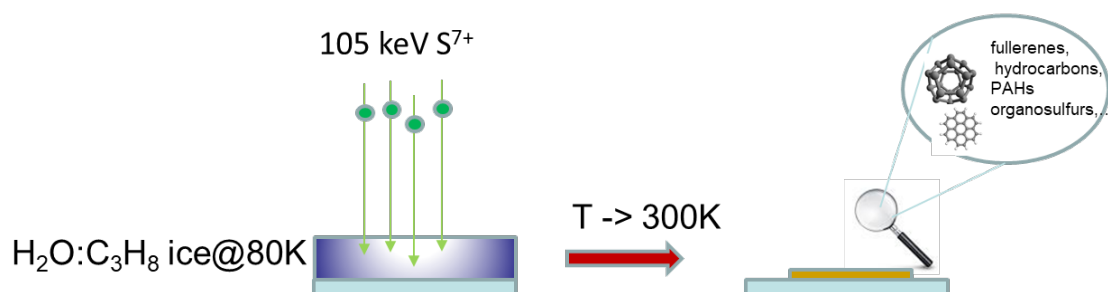
Figure 1: Sulfur ion implantation into water-alkane ices.

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Photo-processing of carbonaceous dust grains by water ice

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The chemical interactions between dust and oxygen-bearing ice have been investigated in experimental studies including vacuum ultraviolet and cosmic-ray processing. The erosion of carbon grains induced by X-ray irradiation of H2O ice was systematically studied in a recent series of experiments. A better understanding of the reaction mechanism using selectively isotope-labeled oxygen/carbon species in kinetic analysis was achieved. Interstellar ice/dust analogs were processed by energetic photons at a temperature of ∼13 K. Processing of the ice/dust interface led to the formation of CO_2, which further dissociated to form CO. Carbonyl groups were formed by oxygen addition to grain surfaces and were confirmed as intermediate species in the formation process.

Effect of gamma radiation on structure, morphology, and optical properties of GO/PVA nanocomposite

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Carbon derivatives, such as graphene and graphene-based compounds, have garnered much attention in recent years due to their distinct features. Batteries, supercapacitors, catalysis, sensors, electronics, and other applications rely on these chemicals. It was specifically chosen for its capacity to function as an electrode in supercapacitors. The produced GO/PVA composites with GO concentrations of 1 wt% and 5 wt% were subjected to gamma radiation at various dosages (1, 50, and 150 MRad). Gamma radiation is known to cause structural changes in materials. As a result, understanding how the GO/PVA system's characteristics change in response to gamma radiation is extremely important.

In the XRD pattern of 1 wt % GO/PVA, the intensity of additional peaks increased due to γ radiation. The reason for this is that due to the breaking of hydrogen bonds and separation of GO particles, the polymer easily fills between these layers and creates a new oriented structure [1]. A new peak at $2\theta = 25.40°$ is observed in the pattern of irradiated samples with a dose of 50 and 150 MRad. We think that the reason for observing this peak is the wrinkling and folding of the GO sheets with the increase in the dose. XRD patterns of GO/PVA composite with 5 wt % GO after exposure to gamma radiation at 0, 1, 50, and 150 MRad doses. The structural changes are similar to the GO/PVA composite with 1 wt % GO. Here, the greatest intensity is observed in the XRD spectrum of the sample exposed to radiation at a dose of 50 Mrad.

TEM images show that GO is wrinkled under the influence of γ radiation. From the EDS results, we can see that oxygen is reduced under the influence of γ radiation. Comparing the composites, we can see that the value of the band gap decreases as the concentration of GO increases. Also, the band gap in GO and nanocomposites decreased due to the generation of free radicals and the reduction of oxygen from the effect of radiation. GO/PVA nanocomposites with tunable optical properties may open a new horizon for polymer-based optoelectronic devices.

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Fullerenes as versatile catalysts in prebiotic reactions

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Fullerenes are abundant in the interstellar medium (ISM) [1-3] and are even hypothesized to be the earliest progenitor of life [3]. The formation route of prebiotic molecules have been demonstrated in Miller-Urey experiments. In this study we theoretically investigate the catalytic effect of fullerenes on Miller-Urey chemistry.
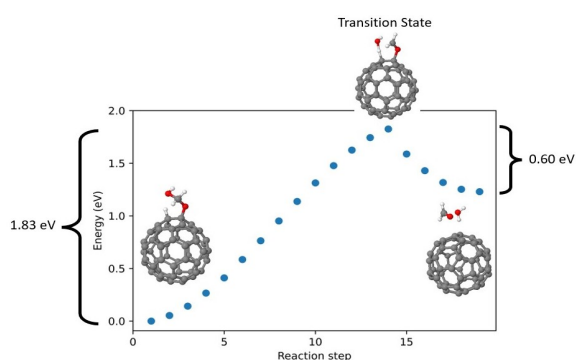
Figure 1: Reaction kinetics of methanediol dissociation to formaldehyde and water. The C_{60} acts as a catalyst by reducing the reaction barrier from 2.32 eV to 1.83 eV.

The kinetics of various reactions in the presence of C_{60} are studied by using *ab initio* calculations. The reaction barriers are calculated with and without the presence of the C_{60}. In our first reaction, we synthesize CO and [O] from CO_2. In our second reaction, we synthesize CH_2O and H_2O from CH_4 and 2[O], by finding an intermediate step of $CH_2(OH)_2$. In our third reaction, we synthesize HCN and H_2O from CO and NH_3. In our fourth reaction, we synthesize HCN and $3H_2$ from CH_4 and NH_3. This process is known as BMA or Degussa [22] process in the presence of a platinum catalyst. We compare the catalytic performance of fullerene with platinum in this reaction.

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Low-temperature photochemistry of sulfur-containing complex organic molecules.

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Sulfur-containing molecules exist in various astrophysical environments and play an essential role in biological systems. We performed *ab initio* quantum-chemical computations and low-temperature photochemical experiments on the selected organic thiols, sulfides, and thiocyanates to understand their reactivity and evaluate the existence of sulfur-containing complex organic molecules in the interstellar medium, especially in the UV-reach environments.

We used broadband vacuum UV light with intensity maxima near Ly-α and excimer UV lasers to irradiate a sample of CH_3SH [1], C_2H_5SH [2], CH_3SCH_3 [3], $HSCH_2CN$ [4], CH_3SCN [5], CH_3NCS [5] embedded in carbon monoxide and argon ices. Using infrared and luminescence spectroscopy, we detected several products, usually much smaller than the irradiated molecule. The OCS is the only product detected that formed due to a reaction with carbon monoxide.

Ab initio quantum chemical computations use a hierarchy of the coupled-cluster wave functions and Gaussian basis sets to deliver knowledge on the potential energy surfaces [1-6]. We identified the most thermodynamically stable isomers and showed that the S-H and S-C bonds can easily be broken upon electronic excitation.

Although more data are needed, we suggest that thiols including C_2H_5SH, can exist only in interstellar clouds well shielded from UV radiation like G+0.693-0.027 but not in Orion KL.

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Electronic and optical properties of molecules calculated within DFT based schemes: from PAHs to nucleobases

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In recent decades, we have used various computational techniques and schemes to determine the electronic properties and absorption spectra of several molecules that are significant for astrochemistry research. Specifically, we focused on the polycyclic aromatic hydrocarbons (PAHs) and the RNA/DNA nucleobases. PAHs are among the most abundant molecules in space, after molecular hydrogen and carbon monoxide. They play, therefore, a fundamental role in the Photophysics of the Interstellar Medium (ISM) [1]. Studies have shown that meteorite samples contain nucleobases. Hence, these informational components of RNA/DNA could have contributed to the development of life molecules on Earth in the past [2].

Different computational methods using density functional theory (DFT) have been employed at our laboratory to calculate the optimized ground-state geometries of these systems. Electronic absorption spectra and excitation properties were evaluated using time-dependent implementation of DFT (TD-DFT) and DFT in the Random-Phase Approximation (DFT-RPA [3-5]. DFT total-energy differences enabled us to evaluate the electron affinities and first and second ionization energies in the case of PAHs but also the one-particle correction to the HOMO–LUMO gap through the D self-consistent-field (DSCF) scheme [3,4]. Two-particle effects in the spectra could be evaluated using either the DSCF scheme or the Bethe-Salpeter-Equation (BSE) method [3,6]. We calculated the electronic properties for ground and excited states of free PAHs. We considered neutral and ionized states as well as the effects of substitutions [3,7]. We also considered free or adsorbed nucleobases on solid surfaces [5,8]. The research results will be presented for some members of the PAHs and of the nucleobases.

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Fullerene derivatives from single metal atoms to molecules: A quantum chemistry perspective

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The well-known presence of fullerenes (C_{60} and C_{70}) in astrophysical environments has strongly increased the motivation to search for fullerenes derivatives in space. In particular, those formed by C_{60} and species already detected in the interstellar (and circumstellar) medium like metal atoms and small organic molecules. Speculatively, both metals and molecules could react with fullerenes in order to produce more complex species like metallofullerenes and fullerene adducts. The extraction of infrared (IR) spectral information from laboratory data about these fullerene derivative species has been a challenging task for astrochemists. In this sense, the predictions from quantum chemistry calculations can give us interesting insights on the formation and the spectral fingerprint of these complex fullerene species; something that can be used to reveal their possible implications in astrochemistry. The present theoretical study focus on fullerene adducts composed by C_{60} and some small polycyclic aromatic hydrocarbons (PAHs) known to be present in space (e.g., indene and naphthalene, among others) and their different IR spectral characteristics compared with other fullerene derivatives like metallofullerenes. Contrary to general expectation, PAH-fullerene adducts display a peculiar IR spectral fingerprint, very different from the metallofullerenes one that preserve the four strongest pristine IR features of C_{60}. The main reasons for such IR spectral differences are discussed and some simulations of the IR emission from these fullerene species under astrophysical conditions are presented.
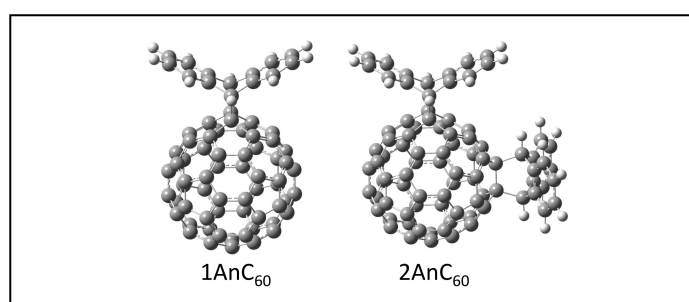

Figure 1: Optimized structures at the DFT B3LYP-D3/6-31G level of PAH-adducts from: (a) mono-anthracene ($1AnC_{60}$) (b) bis-anthracene ($2AnC_{60}$)

Almost Complete Classification of Carbon Molecules based on their Conductivity

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The source and sink potential (SSP) model describes ballistic molecular conductivity. Introduced by Ernzerhof et al in 2004, the SSP model predicts the fractional transmission T (E) of an electron through a hydrocarbon or carbon molecule as a function of energy E [1–17]. The molecule with two prescribed connection carbon (C) atoms (terminals) forms a molecular electronic device (MED) connected in a circuit by two semi–infinite wires across a small bias voltage [18–22]. A graph theoretical treatment considers the 0–1–adjacency matrix A of the molecular graph which is the C–framework where the edges are the C–C sigma bonds. The molecules are π−systems, that is each C atom of the neutral (uncharged) molecule contributes a delocalized electron. These are the electrons which may produce a flow of electricity through the molecule. The number of non–bonding orbitals in the molecule is the nullity of A [23–28]. The rational function T (E) involves the characteristic polynomials of the molecular graph and three of its subgraphs that depend on the connection vertices. The transmission T (0) at the Fermi level of energy leads to selection rules that distinguish 11 possible cases depending on the nullities of the molecular graph and its three subgraphs. The presence of the delocalized electrons may lead one to expect all MEDs to be conductors. This is not the case. A molecule conducts or acts as an insulator depending on the underlying molecular graph and its connection atoms. We showed that in general, a molecule can change its transmission properties from conduction to insulation by using appropriate connection atoms for the desired electrical behaviour [29–30]. Most molecules exhibit mixed (X) conductance. However we showed that omni–conducting (C) and omni–insulating (I) molecules exist. In these molecules the electric behaviour is independent of the connecting atomic terminals [31–34]. A refinement of the selection rules leads to an almost complete classification. Our goal is that every possible single-molecule, two-lead MED based on the carbon framework of any conjugated π system has its place within the structure. The terminals are taken to be at an odd distance, a non–zero even distance or the zero distance apart. The electrical behaviour depends on whether the nullity of the molecule is 0, 1 or more than one [35–42]. The electrical behavior is expected to be omni–conducting (C), omni–insulating (I) or mixed (X). The combinations of the electrical behaviour and the nullity type for the three different distance categories give 81 possible cases. We have proved that 42 cases are mathematically impossible. Examples of molecules populating another 35 cases have been found among relatively small molecular graphs. Only four cases remain open to be solved [43].

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Topological data analysis of fullerene graph spectra

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A fullerene graph is a 3-regular, 3-connected, plane graph with only pentagonal and hexagonal faces. Its spectrum is the spectrum of its adjacency matrix. For a graph F_n on n vertices, its spectrum can be considered as a point in n-dimensional space. For a given number of vertices n, we compute spectra of all fullerene isomers on n vertices. The resulting n-dimensional point set serves as the vertex set of a geometric graph $G(n,d)$ obtained by connecting all points whose distance does not exceed a given positive parameter d. We analyze the properties of such geometric graphs, in particular, the evolution of their number of edges and connected clusters with increasing values of d.

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Cosmic nanocarbon inventory database proposal: A sustainable, open-access and open-source Science 4.0 platform

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The goal of the COST action CA21126 - Carbon molecular nanostructures in space (NanoSpace) Working Group 1 is to create a cosmic nanocarbon inventory database. Some existing databases have problems commonly or separately. Some of those problems are creating a database only for the database maintainers' research group's needs, being not up-to-date and remaining inactive, having no database management system (DBMS) in their technical back-end, having no content management system (CMS), being technically archaic since being in the same generation with the World Wide Web's first years, not having a contemporary or truly applied user interface (UI) and user experience (UX). Hence, our suggestion is not to create a *yet another scientific database*, but a sustainable, transferable to the next generations, adoptable to the scientific developments, citable, open-access and open-source Science 4.0[1] platform.

Our proposal considers the editorial, moderation, interface teams/user groups and approved contributors. The database structure allows the user groups of the platform to be designed in an adoptable and sustainable way. Every single contributor of a certain molecule item will be displayed as an author, every single molecule item will be citable separately and will have a DOI number. Every single version of the molecule items will be preserved and accessible. The properties of the molecules can be classified under four main headings: theoretical, computational, experimental and observational. Under these classifications, the database can include features such as the molecules' structural properties, bond lengths, angles, geometries, as well as spectral properties such as optical and infrared, reaction kinetics, etc. One can also upload files such as images and computational, experimental, and observational raw outputs. The database can be structured in an adoptable and sustainable way to implement the future scientific developments with ease. Our proposal is to use PostgreSQL as DBMS. In the back-end of the CMS we propose to use Python since its scientific capabilities. In conclusion, an interactive, sustainable, open-access and open-source platform can be designed with the Science 4.0 approach by allowing approved contributors to enter information by considering NanoSpace's wide portfolio of scientists.

Please scan this QR code to view the suggested database structure.
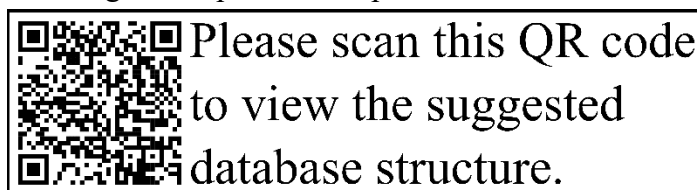
Figure 1: The QR code to view the suggested database structure of the CMS and associated molecular properties. Please scan this QR code or visit
<https://dbdiagram.io/e/65b7e77eac844320aef883e3/65f2dd70b1f3d4062cec570a>.

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Storing and sharing computational data through comprehensive databases

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We have developed a software, ms2simulation, to compute fragmentation spectra simulating unimolecular reactivity by means of molecular dynamics calculations. However, the vast quantity of data generated, ranging from dynamic trajectories to fragmentation mass spectra, presents a challenge in storage and accessibility.

This presentation delves into our approach to address this challenge through the establishment of robust databases. These databases serve as repositories for the extensive data generated by ms2simulation, ensuring its availability to other scientist for further analysis and exploration. We present the outline of the architecture and functionality of these databases, with the aim not only of storing data, but also to facilitate its accessibility and utilization by other scientists.

We will also show the results of similar initiatives such as the SEPIA program database, storing the results of high-level calculation of molecular properties of pesticides, highlighting the importance of centralized repositories in fostering interdisciplinary collaborations.

Atomic Scale Investigations on Nanodiamond Materials via TEM

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Ultrananocrystalline diamond (UNCD) is a crystalline diamond film consisting of 3-5 nm randomly oriented diamond crystallites surrounded by 0.2-0.3 nm wide grain boundaries. These films possess exemplary mechanical, electronic and optical properties [1,2]. Under normal process conditions, these UNCD films are highly electrically insulating, but they can become highly conducting when Ar is substituted in the synthesis gas with some N_2 [1, 5]. In this contribution, we will present the local scale structural and chemical analysis of these n-type UNCD films using aberration corrected and monochromated microscopes [3-5]. These results show where the nitrogen is located into these nanostructures and provide insights into their atomic configuration. These aspects provide very important information about the role played by nitrogen in the formation of such nano-objects. This detailed knowledge is essential for a better understanding of the outstanding properties of such materials as well as for shedding light on their growth mechanism.

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NanoCarbons and how to compute your way out of experimental problems

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Since the start, computer modelling has been a key feature in predicting and rationalizing the peculiar properties of carbon-based nanomaterials and molecules. From our extended experience, applying and developing computational models for these systems, we will discuss available models and how these may be used to yield key information on real-world problems. This will be illustrated in a non-technical way with selected examples from our research, from the mechanism of formation and the structure elucidation of complex Covalent Organic Frameworks (COFs),[1] to synthetic nanographenes,[2] novel doped carbon nanomaterials[3] and bio/nanocarbon composites.[4]
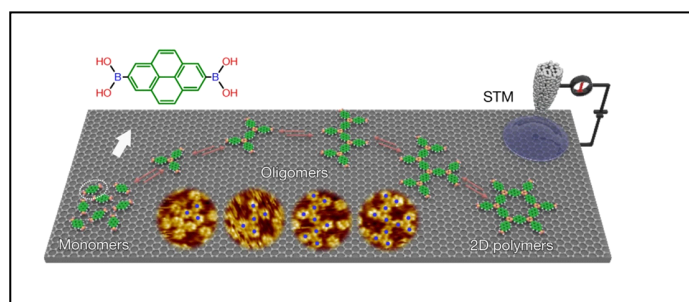
Figure 1: Real-time observation of 2D dynamic covalent polymerization.[1]

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A theoretical study on the mechanisms of formation of primal carbon clusters and nanoparticles in space

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We present a computational study of assembling carbon clusters and nanophases in space from carbon aggregations. Geometry optimizations and Density-functional-based tight-binding (SCC-DFTB) dynamics methods are employed to predict carbon clusters, their time evolution, and their stability. The initial density of the aggregates is found to be of primary importance for the structural properties of the clusters. Aggregates with sufficiently low initial density yield clusters with approximately equal prevalence of sp and sp^2 hybridized states and almost missing sp^3 ones. The increase in the initial density results in sp^2-dominant tangled polycyclic molecules. Larger initial aggregations with tetrahedral interatomic orientation result in sp^2-dominant multi-dimensional polymers. Such materials are highly porous and resemble axially bound nanotubes. Some resultant clusters resemble fullerene building blocks. Spheroid nanoparticles resembling improper fullerenes are predicted by metadynamics, aimed at inter-fragment coupling reactions. Among the studied systems they have the lowest binding energy.
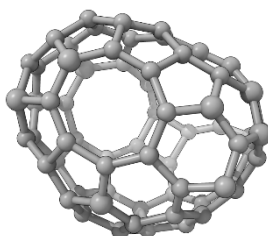
Figure 1: Optimized geometry of the fullerene-like, closed-cage cluster C66.

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Chemical functionalization of Multilayers fullerenes (Carbon nano-onions) for biomedical applications

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In this presentation, multilayers fullerenes, also known as carbon nano-onions (CNOs), will be discussed as a potential vesicle for nanocarrier-type drug delivery systems.1 CNOs, or multi-layer fullerenes, consist of multiple concentric layers of sp2 hybridized carbon and are emerging as platforms for biomedical applications because of their ability to be internalized by cells and low toxicity.2

In my research group we have developed methodology for the synthesis of pure, monodispersed CNOs and various chemical functionalization strategies for the introduction of different functionalities (receptor targeting unit and imaging unit) onto the surface of the CNOs. The modified CNOs display high brightness and photostability in aqueous solutions and are selectively taken up by different cancer cell lines without significant cytotoxicity. Supramolecular functionalization with biocompatible polymers is an effective strategy to develop engineered drug carriers for targeted delivery applications. We reported the use of a hyaluronic acid-phospholipid (HA-DMPE) conjugate to target CD44 overexpressing cancer cells, while enhancing solubility of the nanoconstruct. Non-covalently functionalized CNOs with HA-DMPE show excellent in vitro cell viability in human breast carcinoma cells overexpressing CD44 and are uptaken to a greater extent compared to human ovarian carcinoma cells with an undetectable amount of CD44. In addition, they possess high in vivo biocompatibility in zebrafish during the different stages of development suggesting a high degree of biosafety of this class of nanomaterials.3 Our results encouraged us to further develop them as targeted diagnostics or therapeutics nanocarriers. We successfully loaded the CNO-based nanocarrier with chemotherapeutic prodrugs derived from gemcitabine, and showed remarkable efficacy in killing pancreatic adenocarcinoma cells.4

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Emergent Atomic Environments in Twisted Bilayer Graphene and Their Use in the Prediction of the Vibrational Properties

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While Bernal stacked bilayer graphene bears two distinct atom types in its lattice, there exists no analytical framework addressing the number of atomic environments that emerge in twisted bilayer graphene superlattices. In this work, we have computationally analyzed 120 different twisted bilayer superlattices using descriptor functions to study the emergent local environments. Our study reveals that the number of atoms with unique local environments depend on the superlattice size linearly. Moreover, this linear dependence manifests itself on two distinct lines and this automatically suggests a new classification scheme based on the local environments. As a possible application, the use of local environments in the investigation of vibrational properties is discussed with respect to the existing literature. Molecular dynamics simulations are performed to calculate the phonon density of states of the 120 structures as well as the local phonon density of states of their individual atoms. The similarity of the contributions of local density of states coming from atoms with the same local environment is demonstrated. Local density of states of the atoms with unique local environments of an arbitrary selection of the structures is then used to train a machine learning model. This model is used to predict the phonon spectra of twisted bilayer structures. Performance of the trained model is discussed thoroughly via different selection of training and test sets, and it is shown that the model proves effective in predicting the vibrational properties of any given twisted bilayer structure. The possible applications of the generic method presented which reaches far beyond twisted bilayer graphene is also discussed.

Using Quantum Computer assistance to scale up Quantum Correlation measures for nC

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Fermionic correlation measures are becoming a popular approach in quantum chemistry and condensed-matter physics communities to describe the electronic structure.[1,2] This trend aligns well with the ongoing the push for "second quantum revolution."[3] Such tools require the expertise of both the Quantum Information theory and Quantum Chemistry communities[4]. This perspective on electronic structure holds the promise to model long range emergent networks, photon- and ion-induced heterogeneities and their spectral consequences[5] from first principles; as well as developing novel quantum detector technologies. In alignment with the "second quantum revolution" the approach also allows exploring nano carbon as potent sources of entanglement and quantum correlations, key resources for various quantum technologies. The need for fermionic correlation measures arise from current challenge for quantum chemistry and condensed-matter physics: to understand phenomena where critical phenomena and non-equilibrium dynamics go beyond classical mean field approximations.[6] However, tools of quantum information theory that use classical computing model do not scale in this regime. For example, in tensor-network representations that most efficiently capture the entanglement in the multipartite system, the cost of classically simulating a general quantum circuit by contracting a tensor network is exponential in the treewidth of the graph induced by the circuit[7] which means systems that are more "classical" can have an efficient representation. For restricted classes of systems that are sufficiently unentangled, efficient simulations by tensor networks are possible, but these are not interesting systems in "second quantum revolution" sense. In contrast, systems that are of interest do not have an efficient representation with a classical computer (if it can be represented at all), but, in theory are easy to represent in a quantum computer. However, in the era of intermediate scale noisy quantum computers (NISQ), these higher correlations are the most sensitive to decoherence and thus the output will be hypersensitive to imperfections. The reliability of NISQ quantum simulation is thus most in doubt for exactly those problems we need them for. An approach that combines the advantages of traditional and quantum computing can circumvent this near term issue. This strategy is widely named as "HPC+QPU", where "QPU" stands for "quantum processor unit" and acts as an accelerator in a similar manner to GPU. Preskill laid out a number of examples where this strategy can have advantages such as quantum machine learning.[8] In this talk, I will go over some of the algorithms we are developing in our group with HPC+QPU strategy, in order to scale existing quantum information tools for describing the electronic structure of nano carbon in space.

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Investigating Devices That Measure Nanocarbon Molecular Structures In Space

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It is available in five allotropic modifications: carbon, carbine, fulleren, nanotubes, non-graphite carbon, graphite and diamond. After the discovery of various allotropes of carbon, carbon aroused great interest in the world of science. Carbon- based nano materials exhibit unprecedented physical and chemical properties such as high strength, excellent corrosion resistance, outstanding electrical and thermal conductivity, and stability. There are various methods for measuring nanocarbon structures in space. These include spectroscopy, atomic force microscopy (AFM), laser scattering spectroscopy and thermal conductivity measurements. How these methods are applied in the space environment and their limitations will also be examined. Nanocarbon Structure Measurement Instruments Used in Spacecraft: Spacecraft can carry different devices for the measurement of nanocarbon structures. These devices include remote sensing systems, sampling devices and sensors specific to nanocarbon structures. How these instruments are designed to be space-compatible and how they are used in space missions will be described. A summary of the current state of the art in the measurement of nanocarbon structures in space will be given and recommendations for future work will be made. It will also highlight how the discovery and characterization of nanocarbon structures in space can benefit space exploration and the space industry. In future studies, it is thought that it will help to produce new devices that measure nanomolecular structures for this field.

Metal-semiconductor transition investigation of nanocrystalline silicon carbide under irradiation in space technology

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Silicon carbide has attractive application at various space devices due to the combination of excellent physical and chemical properties. Silicon carbide has an interesting usage in the artificial satellite electronics by virtue of wide band gap (2.2 eV - 3.3 eV depending on polytype). Simultaneously, nanocrystalline silicon carbide has inherently a high melting point (3000 K or more), hardness, chemical and physical resistance. As a semiconductor, nanocrystalline silicon carbide has a functional application at the high temperatures in space technology. Previously, electrical conductivity, permittivity and radiation-induced conductivity (RIC) of nanocrystalline silicon carbide (3C-SiC) reviewed under irradiation [1-3]. However, metal - semiconductor transition and nature of conductivity in the nanocrystalline silicon carbide under irradiation are missing at the past researches. Obviously, it is inevitable that all material exposure various type irradiation at the real application process in the different space devices.

It is clear that, complex impedance spectroscopy method is best technique for the analysis nature of conductivity and metal - semiconductor transition at the materials. For the determination of metal-semiconductor transition of nanocrystalline silicon carbide, impedance measurements scanned at the different temperature under irradiation. Moreover, semiconducting and metal behavior of conductivity of nanocrystal has been investigated at the various temperatures. Nanocrystalline 3C-SiC particles have been comparatively analyzed under neutron irradiation by changing irradiation period and doping elements concentration using impedance spectroscopy. Metal-semiconductor transition in the 3C-SiC nanocrystal were observed at T_{MS} = 250K, 325K and 370K temperatures corresponding to the value of 0.1MHz, 1MHz and 2.5MHz, respectively. It has been found out that, as a result of neutron irradiation period increase, the numerical value of T_{MS} shifts to lower temperature direction. Observed situation, can be explained dangling bonds, neutron transmutation, formation of defects or additional carriers under neutron irradiation. In real terms, the system cannot be explained by the ideal components, and the capacitor is explained by the constant phase element (CPE). It is important to note that, similar situation observed dielectric loss measurements. Looking dielectric loss as a function of temperature, it is clear that the metal-semiconductor transition shifts slightly towards the temperature decrease after the neutron irradiation. Furthermore, neutron irradiation the effects are clearly observed in f(tanδ) ~ f(T) plots at various fixed frequencies.

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Poster Presentations

Enhancing the thermal stability of TiO$_2$-B nanoribbons

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TiO$_2$-B is a titanium dioxide polymorph first synthesised by Marchand in 1980.[1] Its monoclinic crystal structure which, because of its low-density crystal framework, exhibits larger channels and voids, makes it a suitable host for the intercalation of various ions.[2] Like TiO$_2$ polymorphs anatase and brookite, also TiO$_2$-B is a metastable phase and can be transformed first to anatase and then to rutile via an external thermal driving force.

In this work, we investigated synthetic approaches for increasing the thermal stability of TiO$_2$-B nanoribbons. Typically, H$_2$Ti$_3$O$_7$ NRs transform to TiO$_2$-B at a relatively low temperature of 400 °C. As a precursor in this study, two types of H$_2$Ti$_3$O$_7$ NRs were used pristine nanoribbons[3] and nanoribbons coated with a Ce^{4+}-containing species[4]. The phase transformation, H$_2$Ti$_3$O$_7$ $\rightleftharpoons$ TiO$_2$-B, was induced by calcination in air or/and heating in the NH$_3$ atmosphere between 2 h and 6 h. A thin cerium-containing layer at the surface of H$_2$Ti$_3$O$_7$ nanoribbons increased the temperature for the transformation of TiO$_2$-B to anatase by about 200 °C. Analysis of materials' phase composition with Rietveld refinement showed that all materials contain a small amount of anatase, which is the lowest for the material first calcinated in ai. At the same time, the prolonged heating in the NH$_3$ atmosphere increased the amount of anatase. As revealed by HAADF STEM images visible Ce atoms at the surface occupy mainly regular Ti positions.

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Action spectroscopy of CN containing PAH cations

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The detection of cyano-group containing aromatic structures such as benzonitrile, cyanonaphthalene and cyanoindene in interstellar clouds by radioastronomy [1,2,3] has motivated recent laboratory investigations into their stability. Experiments at the DESIREE storage ring revealed that relatively small polycyclic aromatic hydrocarbon cations may be more stable than previously believed, attributing this to inverse internal conversion and recurrent fluorescence [4]. This has motivated us to obtain the electronic and vibrational spectra of these species to facilitate searches for them in other wavelength ranges. In this poster recent experiments results, obtained by action spectroscopy in a cryogenic trap, will be presented.

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Machnine Learning Methods for DFT simulations of nanostructures

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We discuss the application of data-informed machine-learning (ML) methodology, as part of multi-scale materials simulations based on quantum-mechanical models at the level f Density-Functional Theory (DFT) [1]. The datasets are (1) DFT energies for a variety of nanostructures that have been produced by extensive simulations and (2) experimental data for electronic band gaps that have been collected via systematic searches in the literature. As expected, the calculated total energies are very well reproduced by ML (left panel of Fig. 1), while smaller accuracy is found for the more demanding electronic properties, such as the band gap (right panel of Fig. 1). For both datasets, ML performs extremely well, providing results with mean average errors of the order of tens or hundreds of meVs, and can be used as a valuable tool for materials simulation and materials design.
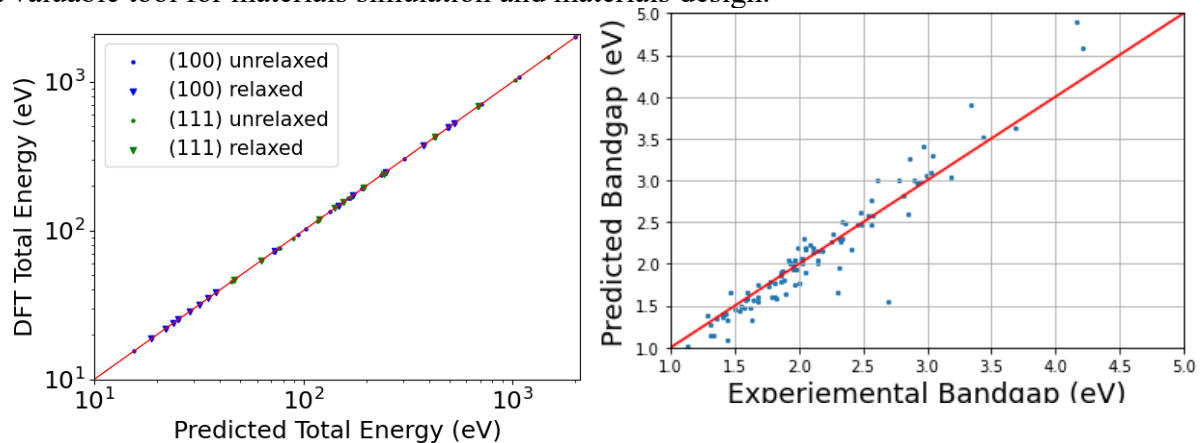

Figure 1: Left: Predicted vs calculated energy for a variety of gold nanoparticles. Right : Redicted vs. Exeperimental band gap for a variety of inorganic nanomaterials.

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Dimeter on Nanotori

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A cubic graph which has only hexagonal faces, and can be embedded into a torus is known as generalized honeycomb torus or honeycomb toroidal graph, abbreviated as nanotorus. This graph is determined by three parameters $a, b,$ and c, and denoted by $G_{a,b,c}$.

Recently, B. Alpspach dedicated a survey paper to nanotori, wherein a number of open problems are suggested.

In this article we deal with one of the problems given in the survey, i.e. we determine the diameter of nanotorus $G_{a,b,c}$ as a function of the parameters $a, b,$ and c. We obtain that the diameter of $G_{a,b,c}$ for $b \leq a$ is just a. For the case $a < b$, we distinguish two subcases: $a \leq c < b$ and $c < a < b$. In both subcases we determine the diameter for b big enough.

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Theoretical and EIS investigation of the formation of oxygen on the hematite surface

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Solid surfaces can gather gas bubbles via processes such as direct immersion in water, temperature or pressure fluctuations, solvent exchange, microwaves, ultrasounds, cosmic rays, and (photo) (electro)chemical gas evolution reaction[1-3].

In this study, a pathway for ion transport between oxygen bubbles and (semi)conducting catalysts was found. To comprehend how bubbles affixed to catalysts affect crucial gas-evolving events in nature and technology, it is critically necessary to identify this portal. This urgency is heightened by the harmful effects that trapped gas bubbles play in catalysis, such as reaction inefficiency and overpotential. As a result, the dissemination of these discoveries to the broad audience of Nature Chemistry will aid continuing study in this fast advancing field of catalysis.

Here, we demonstrate that metal alkali ions restricted to the EDL area of the surfaces of oxygen bubbles may be transferred to and from the EDL of hematite surfaces. Controlling the amount and polarity of an externally applied electric potential traveling through hematite permits direct control of this gateway. Specifically, a negative electric potential enhances ion transport through hematite, whereas a positive electric potential inhibits it. In addition, we demonstrate that ion transport is inhibited when bubbles formed on a catalyst are transferred to an insulator, such as polytetrafluoroethylene.
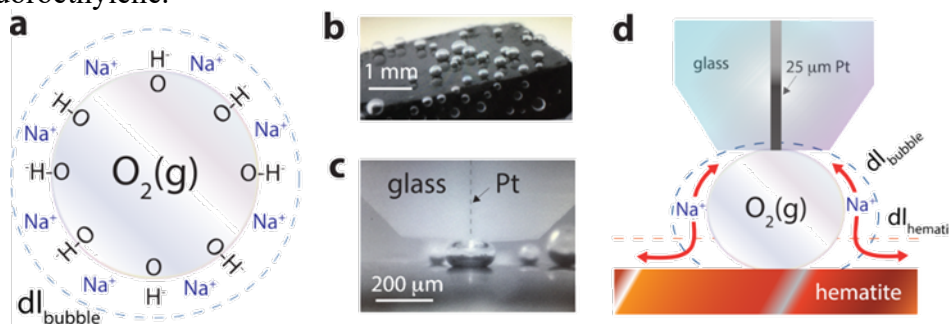
Figure 1. O_2 microbubbles produced and measured electrochemically.

In this investigation, the findings of theoretical MC and MD calculations for the experiments conducted in the study are reported. This is done to evaluate the effect of the electrolyte on the early stage of bubble formation, the adsorption of oxygen on the surface.

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Structure and spectroscopy of molecules of astrochemical interest and their aggregates with water

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Introduction: The first detection of an aromatic molecule in space was made in 2001, when benzene was identified in a protoplanetary nebula.[1] More recently, in 2018, the benzonitrile molecule was the first nitrogenous aromatic cycle detected in the interstellar medium (ISM).[2] In early 2021, the detection of 1- and 2-cyanonaphthalene was reported.[3] These findings confirm that nitrogenous polycyclic aromatic hydrocarbons (NPAHs) are a component of the interstellar aromatic inventory. Both in the ISM and in different astronomical environments, NPAHs can form aggregates with small molecules such as water, which alters their spectroscopy and their photophysical and photochemical properties. Therefore, the laboratory study of the spectroscopy, photochemistry and photophysics of this type of NPAH and their aggregates with H_2O is of great interest in understanding and predicting the chemical composition of the ISM. In this context, we present a study of the spectroscopy of 1-cyanonaphthalene (1CNN) and its aggregates with 1 and 2 molecules of H_2O in the gas phase under conditions of low pressure and temperature to simulate those of the ISM.

Results and conclusions: The generation of 1CNN and its aggregates with 1 and 2 H_2O molecules was carried out by supersonic expansion in a vacuum chamber, reaching pressures and temperatures of the order of 10^{-6} mbar and 30 K, respectively. The REMPI spectrum (1+1') was recorded in the 225-325 nm range, with shifts to lower energies observed for the case of the aggregates with respect to the spectrum of the 1CNN monomer, and signs of evaporation of a water molecule in the case of 1CNN:2H_2O. The ionization energy of the aggregates was determined: 1CNN:H_2O (8.46 eV) and 1CNN:2H_2O (8.40 eV). The excited states of the radical cation form of the aggregates were theoretically studied to evaluate the possible effect of Lyman-α radiation on the photostability and ISM survival of this species. The experimental results showed good agreement with electronic structure calculations at the CAM-B3LYP/aug-cc-pvdz level. The small decrease observed in the ionization energy with the degree of solvation indicates that the effect of the water molecule is similar in the neutral and ionic states of 1CNN.

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Using Concepts of Computer Games Development to Create a Data Visualization Engine

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One of the most powerful aspects of the specialization of software development for the creation of Computer Games is the concept of the Games Engine and their associated Asset Pipelines. By functioning in a highly data-driven fashion they allow the artistic side of games developers to create the custom environments of modern games without much recourse to low-level coding. By borrowing methods from games development and also exploiting off-the-shelf engines (UNITY) we have produced a range of visualizations of general networks as well as nano-molecules across a range of platforms: VR, PC, steam deck, Android mobile phone.

These can heavily borrow from the accepted UI of modern games to produce easily navigable visualizations of especial use to out reach programs.
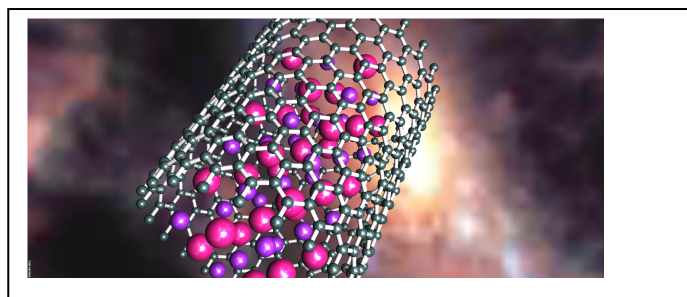

Figure 1: Example of a nano-molecule visualized using the UNITY game engine displayed on a mobile device.

STM observation and characterisation of azafullerene radicals

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Azafullerene $C_{59}N$ is an organic radical, which is analogous to fullerene but one C atom is replaced with N. Since it can be chemically synthesised with a high yield, it is expected to be qubit particles for quantum circuits [1]. However, a remaining challenge for practical application is the stabilisation of $C_{59}N$ radicals in order to avoid re-dimerisation into non-radical dimer $(C_{59}N)_2$ [2].

In this study, we deposit $C_{59}N^\bullet$ radicals on the Au(111) substrate, which interacts, but avoids forming a covalent bond with $C_{59}N^\bullet$. The thickness of $C_{59}N$ film is adjusted to 0.35 – 2.1 monolayers (ML) and each layer is characterised using X-ray photoemission (XPS) and X-ray absorption fine structure (NEXAFS) spectroscopy and scanning tunnelling microscopy (STM), with theoretical supports by density functional theory calculations (DFT) [3].

NEXAFS measurements reveal the molecular orientation of $C_{59}N$ at each layer thickness. We also investigate radical population by utilising the singly unoccupied $C_{59}N$ orbital (SUMO) as a fingerprint of the radical state at each layer thickness. Up to 1 ML, the $C_{59}N$ molecules are stabilised with the radical orbital on the C (adjacent to the N) pointing toward the Au surface and the radical intensity is suppressed. In contrast, the film thickness between 1 and 2 ML shows the large SUMO peak, which indicates an intermediate high-spin-density phase. As the 2nd layer completes, the direction of N atom from the cage centre is almost horizontal along the substrate and the SUMO peak almost disappears, suggesting the $C_{59}N^\bullet$ formed non-radical dimers. We discuss the $C_{59}N^\bullet$ stabilisation on the Au-contact layer, which can be explored for stabilisation and positioning of various molecular radicals on a substrate.

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STM Studies of C_{60} Cage Shrinking on Cu(111)

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When C_{60} (or any other fullerene) is excited in the gas phase via multiphoton laser excitation or relatively low energy collisional excitation, a typical fragmentation mass spectrum shows a series of smaller fullerene fragments, each separated by the mass of a C_2 molecule. The accepted inferred mechanism to form these smaller fullerene fragments is a Stone-Wales bond rearrangement to produce a less stable isomer with adjacent pentagons, providing a lower energy pathway for emitting (or absorbing) C_2. Here we provide evidence from STM/STS experiments for such a fragmentation process undergone by C_{60} deposited on a surface at liquid He temperature where the C_2 is emitted, leaving behind successively smaller fullerene cages on the surface. This may have consequences for understanding the origin of the wide range of fullerene species observed from the Almahata Sitta (AhS) polymict ureilite meteorite [1].
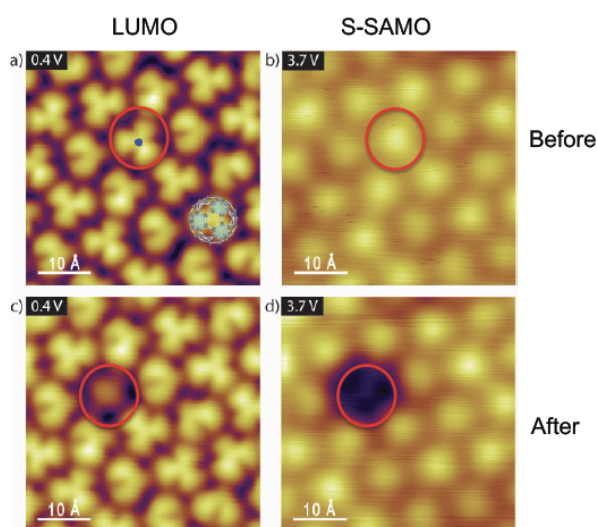

Figure 1. UHV STM images of C_{60} monolayer before (upper) and after (lower) decomposition of the targeted molecule (red circle) by ramping up STM current. The images are of the valence LUMO and Rydberg-like S-SAMO molecular orbital in both cases.

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EiBI Gravity-Modified Solar GES Structure

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In the post-Newtonian era, the Eddington-inspired Born–Infeld (EiBI) gravity theory, considered as an important classical modification of the Einsteinian general relativity formalism, has enabled us to study astroobjects in light of the cosmologically moderated gravitational effects [1]. This EiBI theory imparts a new shape to the usual gravitational Poisson equation through the addition of a cosmological correction factor (EiBI gravity parameter). The main significance of this parameter is in deviation from the Newtonian gravity realized in the form of the system stabilization (destabilization) if positive (negative). A systematic inclusion of this gravity in the basic solar structure equations could lead to a realistic picture of the existing solar models free from end-stage singularity of any kind [2]. A theoretic model is accordingly proposed to investigate the effects of the EiBI gravity on the Gravito-Electrostatic Sheath (GES) formalism of the entire equilibrium solar plasma structure. This study shows that the GES-based solar plasma dynamics is noticeably modified against the previously reported Newtonian GES-model analyses [3]. Here, an equilibrium bounded solution for the solar self-gravity shows the EiBI-modified solar surface boundary (SSB) to exist at a helio-centric radial location $\xi = 4$ (on the Jeans scale). It is found that the EiBI gravity shifts the present SSB outwards by 14.28% relative to the original Newtonian gravity-based SSB. The EiBI gravity effects on diverse relevant solar parameters, such as the electrostatic potential, electric field, and Mach number, are illustratively analyzed. A reliability comparison checkup to validate our investigation in light of the existing solar plasma scenarios is presented, and so forth. It could be anticipated that our exploration could justifiably be used to see the exact equilibrium-fluctuation solar plasma dynamics in realistically modified post-Newtonian gravity environments on both the bounded interior and unbounded exterior solar plasma scales.

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Balancing error and scaling in Quantum Computer with machine learning

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Hamza Korhan, Dr. O. Barış Malcıoğlu

In this poster we summarize our experiments on using AI to balance error rates in

IBM-Q for scaling up the discord calculation problem.

Shaping tomorrow: breaking bias in childhood education

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"Draw A Scientist" is a long-standing sociological test used in schools to examine gender perceptions. Between the ages of 5 and 8, girls mostly draw female scientists. However, the trend reverses around ages 10-11, reaching the age of 16 where female scientists are drawn by only 1 in 4 female students. The majority draw male scientists. (Miller et al. 2018, Child Development, 1943). The decline in interest in scientific subjects among girls occurs with schooling and seems to be caused, among other things, by the different attention that teachers unconsciously pay to male and female students (Leaper & Brown, 2014). Centering on children's education and leveraging the resources offered by their educational influencers, namely parents and teachers, is therefore crucial to addressing the origin of these biases. This approach is not limited to gender biases; it can effectively prevent various forms of discrimination, whether conscious or unconscious, including those stemming from social, cultural, geographic, or religious factors. In this contribution, we will introduce several ideas for crafting educational materials aimed at bolstering the efforts of parents and teachers in raising the new generations.

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Influence of thermal annealing on the physical properties of GO composite materials

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Graphene oxide (GO) is a derivative of graphene that has garnered significant attention. This research involves producing GO using the Hummers method, generating a composite using GO and PVA, and analyzing these composites' structural optical and electrical characteristics. The impact of thermal annealing on the structure and optical characteristics of GO/PVA materials at various concentrations were also investigated. The band gap value changed due to an increase in the concentration of GO in the composites in the PVA and the impact of thermal annealing. The band gap value, specific resistance, and dielectric constant were all found to be well controlled by varying the thermal annealing temperature and the concentration of GO in this case. To study the effect of temperature on the physical properties of GO/PVA nanocomposite materials with different percentages, all samples were thermal annealed at temperatures of 40°C, 70°C, and 110°C. It was determined that at temperatures of 40°C and 70°C, GO formed oriented orientations between PVA layers. At high temperatures, due to the reduction of GO layers under the influence of temperature, the distance between the layers decreased, and at the corresponding temperature, PVA melted and disappeared between these layers. Optical absorption increases with increasing GO concentration in nanocomposites. The band gap value diminishes when the thermal annealing temperature increases. The cause for this is that the polymer's mobility increases as the temperature of thermal annealing rises, making aggregation processes easier. As a result, the size of the particles increases. As a result, the band gap value decreases. The specific resistance of composites diminishes with rising temperatures. As the GO content in the samples rises, the specific resistance decreases. At the same time, the temperature influence caused by structural reorganization within the GO/PVA composite can result in greater alignment and connection of the GO sheets, which optimizes charge pathways and reduces resistance. As a result of the reduction of defects enhances charge carrier mobility and conductivity, resulting in a decrease in specific resistance. At the same time, it is important to study the effect of radiation on GO-based nanocomposite materials. The exposure to gamma radiation-induced structural modifications in the GO/PVA composite film. The radiation caused the breakage of hydrogen bonds, separation of GO sheets, and the incorporation of polymer between the GO sheets, leading to the formation of new cross bonds. Consequently, the diffraction peaks exhibited new features due to changes in bond configurations and the creation of a distinct polymer structure surrounding the GO sheets. It was observed that the band gap value decreased with an increase in the concentration of GO. Therefore, by adjusting either the concentration of GO within the composite, control over the band gap value of the sample could be achieved.

Age-mass ratio and evolution of the herbig AeBe stars

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In this report results of analyzes of the spectral energy distribution (SEDs) in a group of young intermediate mass AeBe Herbig (HAeBe) stars are presented. It is shown that in the group of 19 HAeBe stars, only 3 stars have signs of a remnant debris disks, and its spectrum are classified as type III. The rest of the stars show type II SED curves. The main fundamental parameters and evolutionary status of the sample stars were determined. Only relatively low-mass stars have been found with ages greater than 100 Myr. It is possible more massive stars with ages less than 10 Myr are rapidly losing their circumstellar disks and appear to β Pic and α Lira type stars. Testing this relationship for the rest of the known HAeBe stars (a sample of 311 stars) showed that the relationship exists for the rest of the stars as well.

Keywords: AeBe Herbig stars, circumstellar disks, fundamental parameters