The British Carbon Group

NEWSLETTER **March 2024**

Royce Hub Building, University of Manchester

See www.britishcarbon.org for further details

Contents

Editorial

Samantha Wilkinson, Secretary of the British Carbon Group

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This issue of the BCG newsletter advertises some further details of upcoming Carbon conferences and events, including Carbon 2024 – The World Conference on Carbon on 14-19th July 2024, Shenzhen World Exhibition & Convention Center, Shenzhen, China. The BCG is still accepting Brian Kelly award nominations. The award is intended as a travel grant (£750) for students and early career researchers with up to 10 years of postdoctoral experience to attend the annual World Carbon Conference. Anyone living or working, at the time of that conference, in the country where the conference is held is not eligible. As a consequence, applications will not be accepted from China on this occasion. For more information on how to apply please visit the website:

https://britishcarbon.wordpress.com/2022/03/11/the-brian-kelly-award/

The closing date for applications is the 1st May 2024. Below there is also further information on the British carbon group early careers event and AGM. Finally, this edition of the newsletter rounds off with a very interesting article relating to carbon in space.

Future Event : Carbon Science and Technology: Early Career Researchers Meeting

4th June 2024, Royce Hub Building, University of Manchester, UK

The British Carbon Group is pleased to invite you to their latest event – a day of early career oral and poster presentations at the Royce Hub Building, University of Manchester, UK at 10:00 4th June 2024. It will also feature this year's Ubbelohde Memorial Lecture and the group's Annual General Meeting. The event include:

- Carbon research oral presentations by early career researchers
- Ubbelohde Memorial Lecture by Professor Rahul Raveendran Nair, University of Manchester
- Poster competition with the winner receiving £100 Amazon vouchers
- Buffet lunch

This event is free but registration is required, and send an abstract if you would like to be considered for an oral or poster presentation, by emailing BCG committee member Samantha Wilkinson by 30th April:
Samantha.wilkinson@uknnl.com

Abstracts should be max. 500 words. Poster presentations should be A1 size. Oral presentations will be 15 mins + 5mins Q&A.

Please speak to a member of the BCG committee if you would be interesting in joining the committee.

Future Event : 7th EDF-Energy Nuclear Graphite Conference

6-9th May 2024, Manchester

Manchester Conference Centre at The Pendulum Hotel, Sackville Street, Manchester M1 3BB *(5-minute walk from Piccadilly Rail Station)*

To be held in the ***Momentum Theatre***

Tuesday 7th – Thursday 9th May 2024

http://graphitecore.pro

ABSTRACT SUBMISSION DEADLINE: MARCH 15th
REGISTRATION DEADLINE: APRIL 12th

"MANAGING THE FULL LIFE CYCLE OF A REACTOR WITH A GRAPHITE CORE"

The previous EdF graphite conferences have been primarily held to showcase the high level of supportive technical and scientific work which has allowed the British Advanced Gas-Cooled Reactors (AGRs) to operate to lifetimes well beyond those originally envisaged. Six high-quality peer-reviewed publications have resulted. This work continues in support of continued operation of the reactors.

All Magnox reactors and some of the AGRs are now in a decommissioning programme and there is a need to devise appropriate dismantling procedures and management of radioactive material, including the moderator and reflector graphite. The theme of this conference will include the work on the disposal of UK nuclear graphite which accounts for 1/3 total inventory worldwide.

Also looking ahead, we can envisage the large experience of UK designers and engineers in contributing to the next generation of Advanced Modular Reactors (AMRs), where designs based either upon the principle of the high-temperature reactor or the molten-salt reactor will utilise nuclear graphite as reflector and/or moderator and, in the case of the HTRs, a stream of carbonaceous waste will be produced from the fuel.

We therefore invite contributions in all nuclear-graphite areas (decommissioning, continued operation and future reactors) and look forward to welcoming many scientists and engineers working in the field to Manchester!

Presentations are therefore invited in the following 'nuclear graphite' categories:

Maximising AGR Lifetime

Decommissioning Planning and Experience in Graphite-Moderated Reactors

Deploying Experience for the Next Generation of Reactors

Presentations: will be of 20-25 minutes duration. An ABSTRACT of 100-200 words should be submitted as soon as possible by e-mail to the conference management team at confer@globalnet.co.uk – please write ABSTRACT in the subject line of your mail and attach an Abstract in WORD format using the template to be provided shortly on the website (see below).

Publications: all presentations will hopefully be supported by a technical paper intended for peer-review and publication, as in previous EdF conferences. Papers will be subjected to a thorough independent peer review before being accepted for publication: the publication will be in the style of the previous conference proceedings, published by FESI following the 2018 conference in Kendal (ISBN 978-0-9935485-2-9).

Discussions: moderated discussions have been a fruitful feature of previous conferences and we hope to include similar activities in the 2024 programme.

Delegates are asked to travel to Manchester for the first presentations starting promptly at 13:00 Tuesday 7th May. The conference will finish late afternoon on 9th May.

There will be a **conference dinner** on Wednesday evening, 8th May *(dress code business casual)* – venue: 'Malmaison', near Piccadilly Rail Station.

Future Event : NanoteC 2024

NanoteC is one of the longest running series of international nanoscale carbon conferences in Europe (since 1998). It brings together scientists working with nanoscale carbon materials: nanotubes, graphene, diamond- and fullerene-related nanostructures. This also includes related low dimensional non-carbon based systems, such as transition metal dichalcogenides, among others. While each of these materials attracts its own dedicated community of researchers, NanoteC draws on common themes and allows researchers to share insight into this unique element at the nanoscale.

Elemental carbon shows remarkable variety in properties via simple covalent bonding, however other systems (for example containing nitrogen or metals and low dimensional layered non-carbon based systems) are becoming important and provide alternative components with unique mechanical and electronic properties. Nanotechnology requires an understanding of these materials on an atomic level and this will be the central theme.

The NanoteC conferences are renowned for their relaxed and friendly atmosphere, with emphasis on discussion and participation. We endeavour to achieve as much student participation as possible, and we anticipate that the keynote talks will provide a great dose of inspiration to the next generation of nanotechnologists and surface scientists. It is a four day meeting (three full days of science), with poster session and an evening banquet in Nantes. The following weekend there is a free open-air jazz festival throughout Nantes ("rendezvous de l'Erdre") if you are interested in staying a little longer and taking advantage of that.

Keynote speakers include:

Vincent Meunier
(Penn State, US)

Alexandra Carvalho
(National University of Singapore)

Carla Bittencourt
(University of Mons, Belgium)

If you would like to register please go to the conference website:
https://sites.google.com/view/nanotec24/home

Future Event : Carbon 2024 – The World Conference on Carbon

14-19th July 2024, Shenzhen World Exhibition & Convention Center, Shenzhen, China

Carbon2024 (sz-graphene.ac.cn)

Tsinghua Shenzhen International Graduate School, Shenzhen University of Advanced Technology, and the Institute of Metal Research, CAS, have the honour of organizing The World Conference on Carbon, which will take place in Shenzhen, China, from July 14th to 19th, 2024. This congress is the most important one in carbon science and by tradition it takes place in the America, Europe, or Asia, and this year will be held, for the third time, in China with the support of the Shenzhen Science Technology and Innovation Commission. This conference plans to receive more than 450 abstracts from over 30 countries. It will have 5 plenary lectures, 40 keynote talks, 160 oral presentations, and around 200 posters, of excellent scientific quality, will be presented.

Themes this year are:

Nano carbons: graphene, graphdiyne, CNTs and fullerenes
Graphite, diamond, porous carbon, coal, coke
Carbon fiber and their composites
Carbon for energy storage and conversion
Carbon for environment
Carbon for biology, health, and medicine
Carbon for electronics and optoelectronics

Cosmic Fullerenes

Dr Chris Ewels, BCG Vice-Chair

The science of carbon in space is undergoing a revolution, thanks to unprecedented emerging high-resolution image and spectroscopy data, notably from the James Webb Space Telescope, but also through new breakthroughs in laboratory experimentation and computational modelling. A new European COST project, “Nanospace”, is bringing together scientists from diverse disciplines to explore this further (https://research.iac.es/proyecto/nanospace/). If of interest, you are very welcome to join the project, simply contact Dr Anibal Garcia Hernandez, the Action chair (via the project website). The following brief overview of Cosmic Fullerenes is produced by some of the project members as part of a much larger (>30 article) review and roadmap. This will be appearing shortly (open source so with free access) in the European Physical Journal D. We thank them very much for permission to reproduce here.

Cosmic Fullerenes

J. Cami[1,2], P. Ehrenfreund[3], H. Linnartz[3], A. Manchado[4], E. Peeters[1,2], Nick L.J. Cox[5], C. Ewels[6], J. Bernard-Salas[5], D.A. Garcia-Hernandez[4], E.K. Campbell[7]
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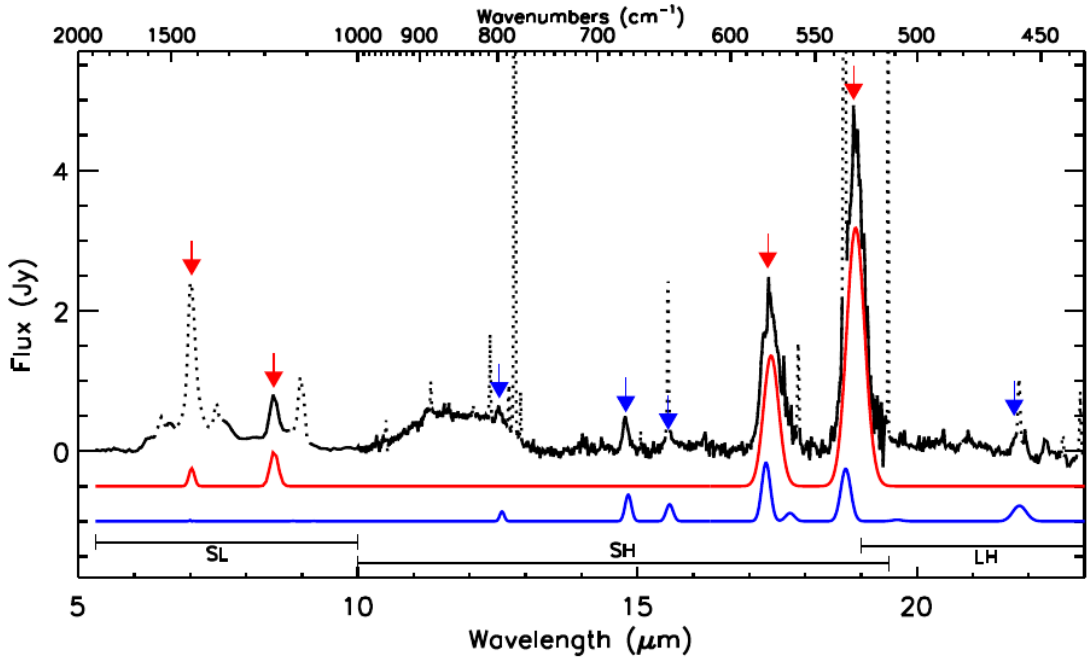
[7]The University of Edinburgh, UK

Ever since the buckminsterfullerene C_{60} was discovered on Earth in experiments simulating the carbon-rich circumstellar environments of evolved stars, they were predicted to be widespread and abundant in the universe [1]. Almost forty years later, C_{60} and C_{60}^+ have been reliably detected and identified in space [2, 3, see also Fig. 1]. Especially the infrared features of C_{60} have been seen in diverse astrophysical environments – from the surroundings of various types of evolved stars to interstellar clouds and to the planet-forming disks around young stars. Fullerenes are not frequently detected however; for example, only a few percent of the C-rich planetary nebulae that have been observed with the Spitzer-IRS spectrograph show the characteristic C_{60} features. When they are seen, their estimated abundance is rather high for a single molecular species – ranging from 10^{-4} to 3% of the available carbon [see e.g. 4, for an overview]. Thus, C_{60} is certainly widespread in space, and when it is seen, it is also abundant. There appears to be only one clear case for the presence of C_{70} thus far [2]. Searches for C_{60}^-, for smaller or larger fullerene cages, as well as searches for protonated or metal-complexed C_{60} compounds have been inconclusive [5–9].



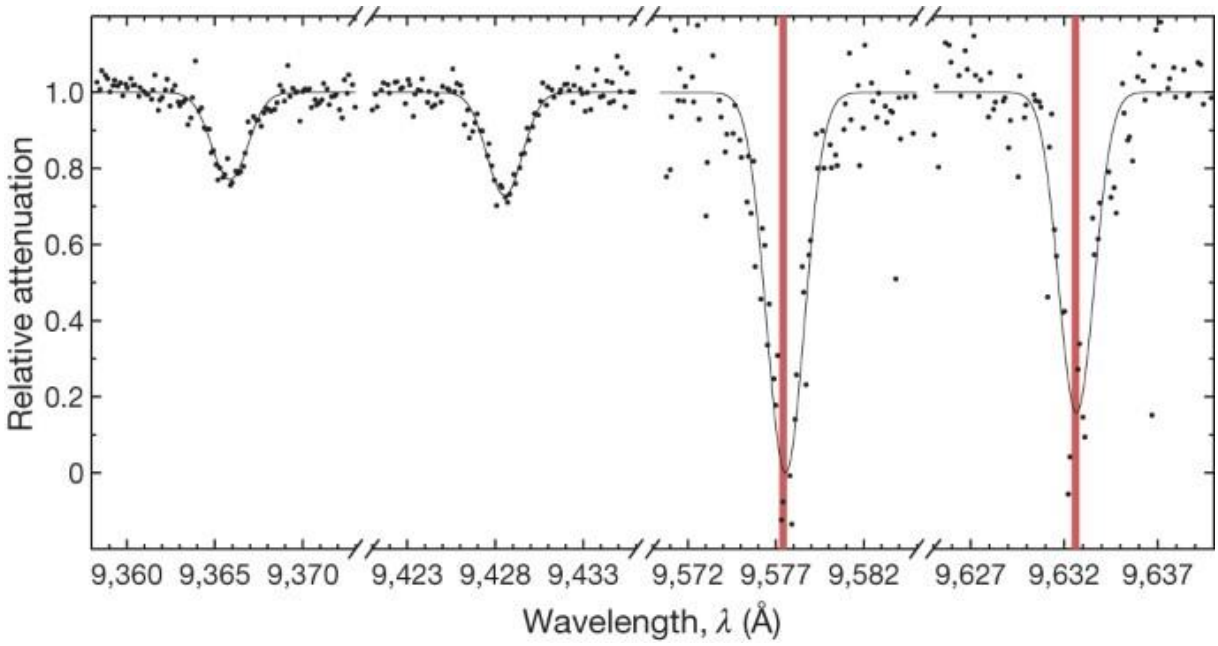


Fig. 1 (top) The continuum-subtracted Spitzer-IRS spectrum of the planetary nebula Tc 1 (black) compared to (thermal) models for C_{60} (red) and C_{70} (blue). Figure taken from [2]. (bottom) Laboratory spectrum of C^{+}_{60} showing clear absorption bands at the wavelengths of the observed diffuse interstellar bands (DIBs) at 9577 and 9632Å. Fig. from [3].

Despite much research since the initial discovery, the inter- and circumstellar fullerene field is still in its infancy, and the full extent of the role and implications of cosmic fullerenes remains a tantalizing mystery.

Why is this research field so important? In recent years astronomical surveys have resulted in the detection of larger and larger species, underlining that we live in a molecular universe, capable of species as complex as C_{60}. This fullerene is also the only identified large aromatic species that has been seen in a variety of objects across the stellar lifecycle. The molecular physics of fullerenes is expected to be identical (albeit with perhaps slightly different parameters) to that of polycyclic aromatic hydrocarbon (PAH) molecules that represent a much larger fraction of the cosmic carbon, and whose IR glow pervades the local and distant universe. However, progress here has been hampered by the fact that the PAH emission represents the combined emission of an entire family of molecular species whose response to the local conditions depends on molecular size, charge state, geometry and precise chemical makeup. This makes it very hard – if not impossible – to critically test theoretical models for the evolution and excitation of large molecules in space. Just like PAHs, C_{60} emission is seen in photo-dissociations regions (PDRs), but in contrast to PAHs, they have clearly distinct spectral features. Detailed studies of C_{60} may thus offer the most critical test possible of our models for the formation, excitation and evolution of large carbonaceous molecules.

What will be gained with further advances? Further advances in the field, aimed to understand the formation mechanisms, distribution, excitation and abundance of fullerene compounds in space will allow us to build a solid foundation to describe the molecular physics and the detailed chemistry that governs these species in various environments. Fullerene studies will pave the way for a more general description of how carbonaceous molecules interact with their environment, and how the environment affects their chemistry. Such a description will be crucial to update our models for the large-scale processes that are driven by these species, such as star and planet formation, and galactic evolution.

Current and Future Challenges

Despite the progress made in identifying cosmic fullerenes, we face several hurdles in our efforts to reach a complete picture. A first one is that we do not have a full inventory yet of the fullerene compounds that are present in space. While C_{60} can have strong emission bands (since it only has 4 IR active modes), other fullerene compounds (with a lower level of molecular symmetry) may be much weaker and thus much harder to detect. Another key problem is that current models for the excitation and charge state of fullerenes do not accurately predict the observed IR spectra [10], indicating that something is missing from our models. Chemical pathways may change pure C_{60} into other compounds including structural variants, as well as hydrogenated or otherwise functionalised species. Subtle molecular physics processes, including complex electronic excited state dynamics, may become important under certain conditions. Finally, a coherent picture of the formation and evolution of fullerenes is sorely missing. Theoretical calculations [11] and laboratory experiments [12] have

suggested that C_{60} can form from dehydrogenation of large PAHs, but it is not clear how this process can explain the appearance of C_{60} in young, low-excitation planetary nebulae while they are absent in their more mature counterparts that sometimes show copious PAH emission. In addition, other fullerene formation processes include the photochemical processing of hydrogenated amorphous carbon grains (HACs) [13] and the shock-heating and ion bombardment induced processing of SiC grains [14]. There are likely multiple formation pathways that are relevant for different environments. Finally, there is a clear relation to the problem of the diffuse interstellar bands (DIBs), since currently the only identified DIBs are due to C_{60}^+. This begs the question what other DIBs could be related to other fullerene compounds.

Advances in Science and Technology to Meet Challenges

To meet the challenges, we need a concerted effort of observational studies, targeted laboratory experiments, theoretical calculations and computational chemistry. Much progress can be expected from detailed studies of C_{60} in different environments with the JWST. Laboratory experiments will not only provide us with state-of-the-art spectra of different fullerene compounds for comparison to optical and IR observations, they are also crucial to measure the reaction rates for various physical processes and chemical reactions. Those are indispensable to update our models. Laboratory experiments simulating astrophysical conditions can aid in understanding the formation mechanisms and stability of fullerene compounds in space. Computational models of astrochemistry will play a pivotal role in simulating the complex interactions of carbon-bearing molecules in various astrophysical environments, guiding observational and experimental efforts and interpreting data.

Concluding Remarks

The exploration of cosmic fullerenes stands at the forefront of modern astrophysics, offering a unique gateway to understanding the cosmic carbon cycle and the complexity of interstellar chemistry. As we navigate the cosmos with cosmic fullerenes as our guide, collaboration between astronomers, chemists, and physicists becomes paramount. The integration of observational, laboratory, and theoretical efforts will unlock the mysteries encoded in these carbon structures, reshaping our comprehension of the dynamic and ever-evolving universe.

This article is based upon work from COST Action CA21126 - Carbon molecular nanostructures in space (NanoSpace), supported by COST (European Cooperation in Science and Technology). It is a pre-print and the final version will be available open source shortly from European Physical Journal D. https://research.iac.es/proyecto/nanospace/

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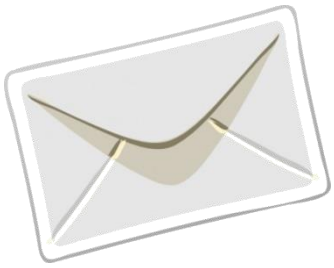
Contact to the Group



The BCG welcomes feedback from its members, so please get in touch with us if you attended one of our events and it sparked an idea, you have been involved in a particularly interesting project or have any other thoughts which might be of interest to the rest of the group!

Please submit any thoughts to samantha.wilkinson@uknnl.com

Items for the next newsletter – Submit an Article

We'd like to hear what you're doing, what you think of the British Carbon Group, any ideas you may have for networking opportunities or anything else you think would be of interest to the rest of the Group. We plan to publish the next Newsletter in Autumn 2024.