Report on the outcomes of a presentation and participation in a ITC Conference[1]

Action number: CA21126

Grantee name: Yuri TANUMA

Conference Details

Conference title: NanoteC23

Conference web-page: https://www.nanotec23.com/home

Conference venue[2]: University of Sussex, Brighton, UK

Conference start and end date: 29/08/2023 to 01/09/2023

Accepted contribution details

Title of the presentation: Nanoscale analysis and theoretical investigation on stable azafullerene radicals protected by carbon nanorings

Type of the presentation: (oral/poster) Oral

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Other details of the presentation: specify here any additional details related to the contribution (e.g. title of the session / track of the conference programme in which the contribution is accepted)

Outcome of the conference participation

Description of the outcome of the presentation of the accepted contribution, in terms of grantee's visibility, including the establishment of new contacts for future collaborations

(max.500 word)

I gave a talk about azafullerene radicals I have investigated so far, i.e., generation of $C_{59}N$⊂[10]CPP radicals by thermal and photochemical treatments, the long spin coherence time of [10]CPP⊃C59N-C60⊂[10]CPP radicals, and the thin film growth of $C_{59}N$. Particularly, the direct observation of $C_{59}N$ film and investigation of growth mechanism by XPS and NEXAFS attracted the attention of other participants.

During the Q&A session, I received a question about STS analysis of $C_{59}N$ molecules. Unfortunately, I could not provide a satisfactory answer since I have not been able to carry out STS analysis of the sample properly due to resolution problem. However, the questioner, a specialist in STM techniques, provided several tips and insights for future during a coffee break after my talk. For example, he suggested placing a platinum area next to the sample so that I can clean the STM tip manually during

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.
[2] For an online conference, specify virtual participation; for hybrid conferences, specify whether it is an in-person or virtual participation.

the observation. We also discussed $C_{59}N$ spin analysis using NV centre and array of active $C_{59}N$ radicals.

For talks given by other participants, there was a young researcher who is studying on theoretical C_{60} clathrates formed by 2+2 cycloaddition by DFT calculations. Clathrates are open-framework structures which repeat the same patterns by sharing bonds with adjacent structures. This caught my interest, because, in the case of fullerene, the inside and out side of the cages coincide. Therefore, I contacted this speaker to explore potential collaboration. My idea is to generate endohedral C_{60} without current high-energy synthesis methods such as the ion implantation and arc discharge. I plan to discuss the C_{60} clathrate structures with him and ask support for quantum calculations of crystal samples, as my experience on DFT calculations is mainly with gas-phase molecules. On my part, I will consider possible experimental setups and conditions, and carry out preliminary experiments.

During the poster session, I interacted a lot of participants including a researcher working on the chemical synthesis of azafullerene with various cage sizes. His group is improving the yield of the products, in addition, he has techniques to attach the azafullerenes on diamond substrate. Therefore, we will collaborate for my future research on spin reading of azafullerene-CPP radical complexes using NV centre. He will prepare azafullerenes and attach them on a diamond substrate with nitrogen vacancies.

I also had the opportunity to talk with a theoretician who is a proficient user of ORCA (DFT calculation software). I am currently using ORCA for my studies on $C_{59}N$ radicals but have encountered issues related to interactions between orbital energy levels when I calculate NEXAFS spectra. Unfortunately, we did not have enough time to delve into this matter in detail due to the public transport problems in the UK, but we will stay in contact and support each other.

Overall, I had a lot of interactions with carbon scientists and fruitful discussions. I sincerely grateful to NanoSpace for providing me with the opportunity to participate in NanoteC23, which resulted in many helpful scientific advises and potential future collaborations.

Acknowledgement of inclusion of necessary supporting documents to claim the grant

I confirm that the following documents have been uploaded on e-COST as an integral part of this report:

- the certificate of conference attendance.

- the programme of the conference or book of abstracts / proceedings indicating the presentation (oral or poster) of the grantee.

- copy of the given presentation (oral or poster).