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

Action number: CA21126

Grantee name: Jorge Diogo Marques Laranjeira

Conference Details

Conference title: NanoteC23

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

Conference venue[2]: University of Sussex

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

Accepted contribution details

Title of the presentation: Understanding C60 Bonding with Computer Models

Type of the presentation: (oral)

Co-authors: K. Strutyński, L. Marques, E. Martínez-Núñez, M. Melle-Franco

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

The oral presentation was met with very positive feedback. The primary focus of the talk centred around the exploration of C60+C60 bonding patterns through computer model. To contextualize this study a brief review of the high-pressure high-temperature synthesis of C60 polymers was presented, as most audiences have limited prior exposure to both high-pressure and high-temperature synthesis of novel materials and the intriguing world of C60 polymers attainable through this methodology.

Consequently, by delving into the motivations behind studying C60 bonding patterns through dimers, the presentation offered the audience valuable insights into these subjects. This was evident in the engaging discussions that followed, as attendees posed questions about the methodologies and the potential they hold.

Moreover, during the presentation, we highlighted our recent work on C60 dimerization and the associated bonding schemes, directing the audience to this valuable resource for a deeper understanding of several innovative bonding geometries we proposed [1].

To further illustrate this, we showcased two previously discovered structures resulting from some of the explored bonding patterns and briefly touched upon their unique properties [2,3].

[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.

In the aftermath of the presentation, we established several promising connections, with potential collaborations on the horizon. These forthcoming collaborations are poised to revolve around the high-pressure, high-temperature investigation of other molecular systems, potentially able to yield novel materials with exciting properties.

[1] J. Laranjeira, K. Strutyński, L. Marques, E. Martínez-Núñez, M. Melle-Franco, C_{60}+C_{60} molecular bonding revisited and expanded, Carbon 213 (2023), 118209.

[2] J. Laranjeira, L. Marques, M. Mezouar, M. Melle-Franco, K. Strutynski, Bonding frustration in the 9.5 GPa fcc polymeric C60, Phys. Stat. Sol. - RRL 11 (2017), 1700343.

[3] J. Laranjeira, L. Marques, M. Melle-Franco, K.Strutyński, M. Barroso, Clathrate structure of polymerized fullerite C_{60}, Carbon 194 (2022), 297.

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)

Applicant enters max. 500 word summary here.

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).