Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA21126 Carbon molecular nanostructures in space (NanoSpace)

Grantee name: Prof Patrick Fowler

Details of the STSM

Title: **Carbon Chemical Graph Theory**

Description of the work carried out during the STSM

Description of the activities carried out during the STSM. Any deviations from the initial working plan shall also be described in this section.

This STSM enabled COST Action members Patrick Fowler (Sheffield) and Irene Sciriha (Malta) to hold intensive face-to-face research discussions on the **chemical graph theory approach to electron structure, delocalisation and flow of electrons within carbon nanostructures**.

Activities were in three parts, as per the working plan.

In Part (I), work focused on preparation of a near-final draft manuscript of a joint paper on Uniform Core Graphs (UCGs). In an exciting development, a proof of the typology of UCGs, which had been a puzzle to us for a year or more, was devised. It turns out that every connected UCG must have least one conduction pair of the type called 11.1 in our paper; this has consequences for the width of the transmission profile for currents through the corresponding molecular device (and incidentally changed the presentation of our paper). A new streamlined version of the ms (with 30 pages,10 figures), acknowledging COST support, was typed up. Subject to independent checking of proofs, reconciliation of ensuing comments via zoom meetings and final proofreading, we are now on track for submission of the ms as a full article to a peer-reviewed journal (e.g. MATCH Communications in Mathematical and in Computer Chemistry) by August 31 2026.

In Part (ii), visiting scientist Patrick Fowler participated in a mini-symposium ‘Symbiosis between Mathematics and Chemistry’ together with three speakers from the University of Malta (Prof. Daphne Gatt (Chemistry, UoM) ‘From molecules to structures: the expanding world of auxetic systems’, James L Borg ‘Distinct vertex-edge spectral labelling for threshold graphs’ and Prof Irene Sciriha (Mathematics, UoM) ‘Nut graphs predict molecular behaviour’, and Patrick Fowler (Chemistry, Sheffield, UK) ‘Graph theory in molecular design: the problem of polyhedral carbon-nitrogen cages’). Talks and question session explored common themes, including the relevance of spectral graph theory to COST Action

[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 Grant Holder Manager to verify the grant documents compliance and proceed with the payment.

Nanospace objectives, and the systematic differences between carbon and nitrogen chemistries, which featured, for example, in pioneering computational work by Nanospace member Chris Ewels (Nantes). Astrochemical interest in nitrogen-containing species is increasing, with identification of cyanocoronene in the Taurus cloud, and the known presence of other NPAHs (nitrogen-containing polycyclic aromatic hydrocarbons) in interstellar dust.

In Part (iii) discussions between the visiting scientist Patrick Fowler and local mathematicians (Irene Sciriha, James L Borg and Dr Martha Borg) were directed to future collaboration on topics within spectral graph theory and its applications. Particular effort was directed to a new scheme for the classification of graph vertices, which has proved crucial in understanding graph classes such as UCGs and the nut graphs (which latter class includes some fullerenes, as studied under the Nanospace Action), constructions for nanotube fullerenes that are also uniform nut graphs, and a first exploration of the extension of nut graphs to other eigenvalues (which would carry similar implications for reactivity and conductivity of the associated molecular species. Work in these directions will continue beyond this STSM, and will lead to publications in peer-reviewed journals in the medium term.

Description of the STSM main achievements and planned follow-up activities

Description and assessment of whether the STSM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the STSM. Agreed plans for future follow-up collaborations shall also be described in this section.

From the account above of this short but highly productive working visit, we believe it is evident, that this STSM abundantly achieved its immediate goals and provided a firm basis for follow-up collaboration.

To be specific: The main activity (see Part (i) above) was preparation of results on the theory of uniform core graphs for publication in the peer-reviewed literature. Work under this heading proceeded at pace, and as a result a substantial (30+ pages) manuscript (‘Uniform-core graphs: Omni–Insulating Core Graphs’, by Irene Sciriha, Bableen Kaur & Patrick W. Fowler) is now in the final stages of checking and revision. It is expected to be submitted within the next 90 days to an appropriate peer-reviewed journal, thereby advancing Action Objectives (A) to (C) (See ‘CA21126 Progress Report at 24 months …’) i.e.

(A) To disseminate the research results towards scientists …

(B) To develop a common understanding of ... known properties of cosmic C nanomaterials (nC) ...

(C) To develop and implement (within the Action) new theoretical approaches …

Activities Parts(ii) and (iii) [i.e. the mini-symposium held at the University of Malta, and the detailed discussions with the Malta mathematics group] contributed to objective (A) and (B) directly. They will further contribute to objective (C), as the specific problems discussed will generate new theoretical approaches. As an example, a further manuscript provisionally entitled ‘An alternative definition of core, middle and upper vertices of a graph: implications for molecular conduction’ with authorship Fowler and Pickup (Sheffield) and Sciriha and Borg (University of Malta) is now in preparation for publication, as a consequence of the STSM. This manuscript introduces a new theoretical framework for the discussion of nullity in graphs, based on use of projector matrices and the Moore-Penrose pseudo-inverse.

This report written by Prof P W Fowler, Sheffield, 30 May 2026