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

Action number: CA21126

Grantee name: Dilara Ickecan

Conference Details

Conference title: NanoTec26

Conference web-page: https://www.nanotec26.org/

Conference venue[2]: National Graphene Institute, Manchester, England

Accepted contribution details

Title of the presentation: Local Atomic Environments to Phonons: Machine Learning Potentials for Low Dimensional Carbon Nanostructures

Co-authors: Yunus Emre Okyayli, Dogan Erbahar

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)

Oral presentation scheduled for Tuesday, 1 September 2026, 15:20–15:40, as part of the afternoon technical session of the NanoTec26 conference programme.

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

Participation in NanoTec26 provided an important opportunity to increase the visibility of my research on machine-learning interatomic potentials for low-dimensional carbon nanostructures within an international community working on carbon materials, nanostructures, computational modelling, and related emerging technologies. I presented our work entitled "**Local Atomic Environments to Phonons: Machine Learning Potentials for Low Dimensional Carbon Nanostructures**" as an oral contribution during the conference programme.

The presentation introduced our approach for developing a carbon only MACE machine-learning potential based on a diverse set of local atomic environments in planar, defective, amorphous, and curved sp^2 carbon structures. I presented the validation of the model against DFT reference calculations in terms of energies, forces, equilibrium structures and phonon properties, as well as its transferability to carbon families that were not included in the training dataset. The presentation therefore provided an opportunity to communicate both the current achievements of the work and its

[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.

[2] For an online conference, specify virtual participation; for hybrid conferences, specify whether it is an in-person or virtual participation.

future directions, including defect migration barriers, finite-temperature simulations and further validation of the potential.

Presenting this work at NanoTec26 increased the international visibility of both my research and our ongoing collaborative work. It also allowed me to discuss the methodology, validation strategy and possible applications of machine learning potentials with researchers working on graphene, nanocarbons, atomistic modelling and computational materials science. The questions and scientific discussions following the presentation provided useful feedback and different perspectives that can contribute to the further development of the study.

The conference also created opportunities to establish and strengthen professional contacts with researchers working on related topics. These interactions provide a basis for potential future collaborations, particularly in the areas of computational modelling of carbon nanostructures, machine-learning interatomic potentials, defect-related properties and vibrational analysis. Participation in NanoTec26 therefore contributed not only to the dissemination of the presented research, but also to expanding my international research network and identifying possible directions for future collaborative studies. The support of the COST Action was also acknowledged in the presentation, further increasing the visibility of the Action and its contribution to international scientific exchange.

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 issued by the conference organiser.

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