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

**Action number: CA21126**

**Grantee name: Slađana Đorđević**

## Details of the STSM

Title: (Anti)aromaticity changes in non-adiabatic dynamics trajectories

Start and end date: 08/10/2024 to 13/10/2024

## 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.

*(max. 500 words)*

The project involved several key steps, starting with the selection of molecules and performing static electronic structure calculations using the algebraic diagrammatic construction second-order (ADC(2)) method. These calculations provided essential insights into the excited electronic states of the selected molecules. Following this, a single non-adiabatic molecular dynamics trajectory was run to describe the evolution of the molecular systems as they transitioned between different electronic states upon excitation. Finally, nuclear independent chemical shift (NICS) values were calculated for the ground state and for approximated excited states.

## 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.

*(max. 500 words)*

The project made significant progress in understanding aromaticity in excited electronic states of organic molecules. The excited electronic states of the molecules were investigated using the algebraic diagrammatic construction second-order (ADC(2)) method. Insight into (anti)aromatic character was obtained by calculation of nuclear independent chemical shifts (NICS) indices only for the ground state

[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.

structures. While the calculation of nuclear independent chemical shifts (NICS) based on ADC(2) wavefunctions remains an important objective for further investigation, the project successfully explored the relationship between electron density changes and aromaticity in excited states.

I can conclude that this short STSM was highly productive. I gained valuable new knowledge in areas that were previously unfamiliar to me and developed several ideas for potential future research directions.