Сенату Универзитета у Крагујевцу

УНИВЕРЗИТЕТ У КРАГУЈЕВЦУ
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КРАГУЈЕВАЦ

Извештај о реализованом постдокторском усавршавању

У складу са потписаним Уговором о постдокторском усавршавању, овим Извештајем обавештавам Сенат Универзитета у Крагујевцу о реализованом постдокторском усавршавању.

Др Слађана Ђорђевић је реализовала постдокторско усавршавање у периоду од јануара до марта 2025. године у истраживачкој групи др. Нађе Дошлић на Институту Руђер Бошковић Универзитета у Загребу.

Сенату Универзитета у Крагујевцу прилажем:

- Извештај о постдокторском усавршавању
- Фотокопију пасоша
- Спецификацију путних трошкова и карте

У Крагујевцу,

8. априла 2025. године

Подносилац Извештаја

Слађана Ђорђевић

др Слађана Ђорђевић

Report of the postdoctoral research stay

Dr. Sladana Đorđević spent three months working within the research group of dr. Nada Došlić at the Ruđer Bošković Institute, University of Zagreb, where she contributed to investigations of excited states in archetypal aromatic and antiaromatic molecules, such as benzene and cyclooctatetraene. The research focused on utilizing advanced computational tools, including Bagel and Turbomole, as well as ZagHop, a specialized program developed by the research group. This collaborative work aims to enhance the understanding of the electronic structure and dynamic behavior of these molecules in excited states.

Vertical excitations were investigated for benzene, toluene, *ortho*-xylene and cyclooctatetraene. Franck-Condon geometry for these molecules was obtained with MP2 method and the cc-pVTZ basis and the cc-pVTZ-JKFIT auxiliary basis set using Turbomole. Adiabatic XMS-CASPT2 calculations were performed within the single-state single-reference contraction scheme (SS-SR) and a real shift of 0.5 au, using the cc-pVTZ basis and the cc-pVTZ-JKFIT auxiliary basis set, using the Bagel software. Active space for benzene, toluene and *ortho*-xylene includes six electrons in six orbitals, while for cyclooctatetraene there are eight electrons in eight orbitals active space.

In benzene S_1 (HOMO → LUMO) state, predicted at 5.01 eV, is dark, while the S_2 (HOMO-1 → LUMO, HOMO → LUMO+1) state, predicted at 6.15 eV, is light. Upon methylation of benzene to form toluene, S_1 and S_2 states are light. Those values are shifted to 4.85 and 5.96 eV. When two methyl groups are added, those values are even more shifted, in *ortho*-xylene the corresponding values are 4.93 and 5.86 eV. At 300 K, obtained spectra for benzene is in accordance with the experimental. Available spectra for toluene indicate that the peaks are shifted to higher wavelengths which is in accordance with calculated spectra.

Next step would be to perform non-adiabatic molecular dynamics simulations. These simulations will involve generating trajectories that describe the evolution of molecular systems through different electronic states upon excitation. The simulations will be performed using the fewest switches surface hopping (FSSH) method implemented in the ZagHop program.

A total of 97 trajectories were initiated from the S_2 state of benzene and propagated for 500 fs. The initial coordinates and velocities were derived from the vibrational ground state Wigner distribution, which is the preferred method for sampling gas-phase systems. Approximately 73% of the trajectories returned to the ground state. These trajectories reached the S_1 state within 115 fs, and the S_0 state within 125 fs.

In cyclooctatetraene, S_1 state is predicted at 4.17 eV and the main transition is HOMO → LUMO, while the S_2 and S_3 states are predicted at 5.99 eV with main transitions from occupied orbitals HOMO, HOMO-1 and HOMO-2 to virtual orbitals LUMO, LUMO+1 and LUMO+2.

The simulations of non-adiabatic molecular dynamics of cyclooctatetraene have been initiated and are currently in progress.

The collaboration between the Institute Ruđer Bošković in Zagreb and the Faculty of Science in Kragujevac has been greatly strengthened through this partnership, creating an environment of creativity, innovation, and mutual respect. Working alongside talented colleagues from both institutions has not only broadened my knowledge but also provided invaluable opportunities for research growth. The strong support system and commitment to excellence at both institutions have made this experience truly enriching, and I look forward to continuing our fruitful partnership.

Supervisor

Dr. sc. Nađa Došlić

Ruđer Bošković Institute

Director General

Dr. sc. David Matthew Smith

Ruđer Bošković Institute