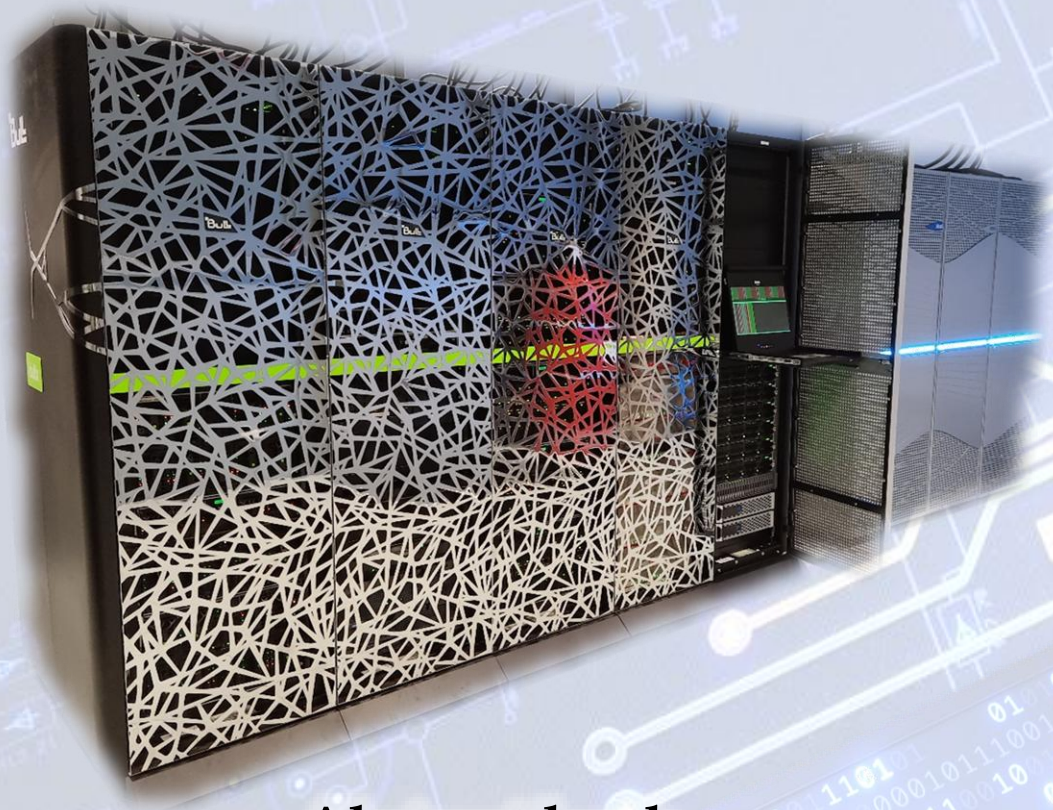
4TH EUROCC VILNIUS HACKATHON & WORKSHOP ON USING HPC



Abstract book

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Carotenoids study Challenges for Modeling Raman and Absorption Spectra

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Carotenoids are naturally occurring pigments with diverse and essential biological functions, particularly in light-harvesting and photoprotection during photosynthesis [1-3]. They contribute to the coloration of leaves, fruits, flowers, and various organisms. The photophysical properties of carotenoids are closely related to those of polyene chains, making them a useful model for understanding excited-state dynamics. Accurate characterization of their excited-state energies and structures is crucial for elucidating the mechanisms of light absorption involving chlorophylls, carotenoids, and related pigments. However, the dynamics observed in Raman and absorption spectra remain incompletely understood [1-3]. Moreover, computational challenges remain in achieving consistency between theoretical predictions and experimental results [4].

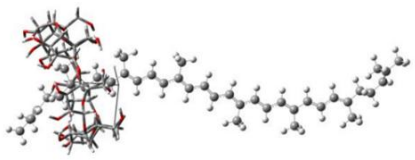

Fig. 1. Lycopene complex with β-cyclodextrin.

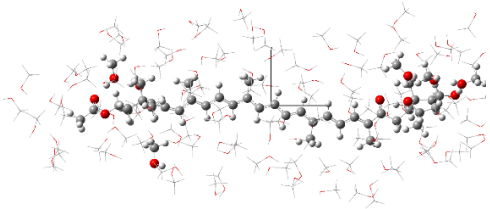

Fig. 2. Fucoxanthin QM/MM simulation

We investigated LYC/β-CD complexes using molecular dynamics (MD) and compared the results with experimental Raman spectra of LYC/HP-CD (Fig.1) [3]. The Raman v_1 band shifts depending on lycopene's position within the β-CD cavity. Using density functional theory (DFT) and ADC(n) methods, we calculated molecular structures, Raman spectra, and excited-state energy diagrams for various carotenoids and polyenes. For fucoxanthin in methanol, MD simulations combined with QM/MM (DFT) reveal a redshift in the lowest optically allowed transition (Fig. 2). The possible supramolecular complexes and their spectroscopic signatures are discussed.

REFERENCES

[1] S. Streckaite, M. Macernis, et al. Electronic and Vibrational Properties of Allene Carotenoids, J. Phys. Chem. A 124, 2792 (2020).

[2] M. Macernis, A. Bockuviene, et al. Raman study for β-ring positioning in β-Carotene complexes with Cyclodextrins and Chitooligosaccharides, J. Mol. Str. 1226, 129362 (2021).

[3] L. Diska, G. Bankovskaite, M. Macernis, et al. Interactions of lycopene with β-cyclodextrins: Raman spectroscopy and theoretical investigation, PCCP, 27 (15), 7874-7881 (2025)

[4] M. Macernis, Component-wise AO Basis Reduction: Norm Loss, Negative Contribution Normalization, and Functional Implications , PCCP, *accepted* (2025)