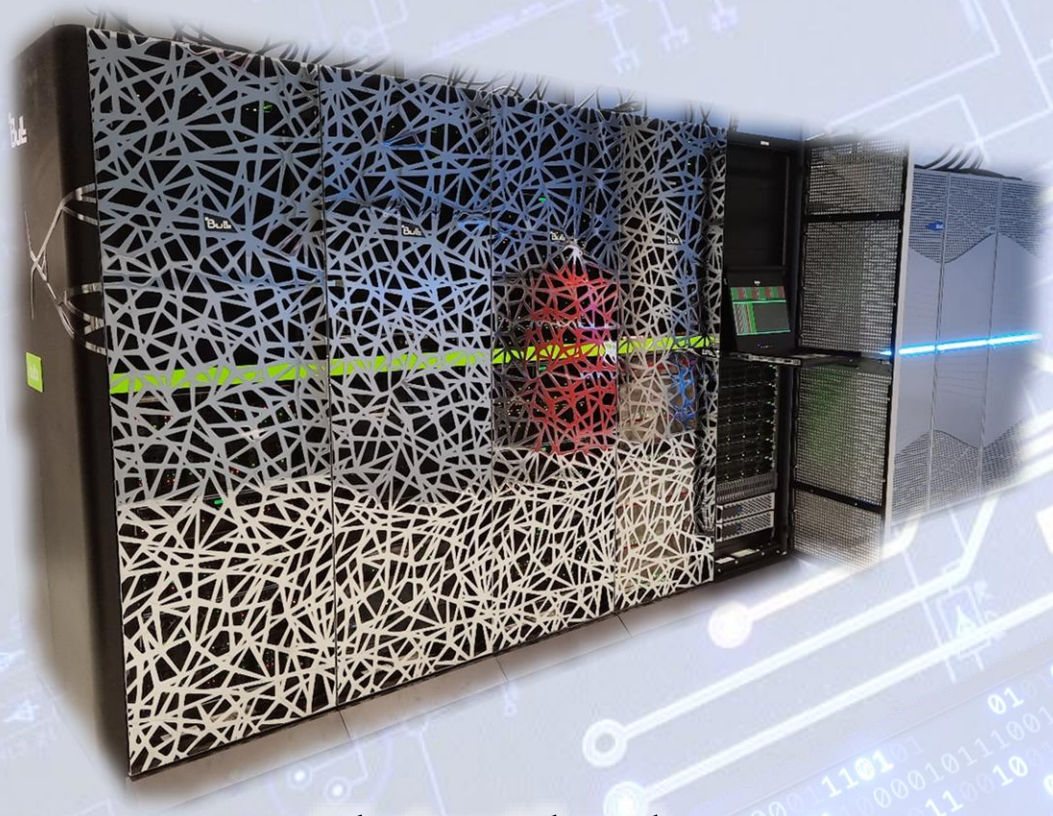
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Modeling Raman and Absorption Spectra of Carotenoids of Various Lengths Using Density Functional Theory and Molecular Dynamics

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Carotenoids are naturally occurring pigments that perform many essential functions in nature [1,2]. They play a critical role in photosynthesis, performing light harvesting and photoprotective functions. Carotenoids are responsible for the coloration of leaves, fruits, flowers, and other organisms. The photophysics of carotenoids can be understood by examining polyene molecules. The study of carotenoid excited-state energies and structures is necessary for a deeper understanding of light absorption processes driven by chlorophylls, carotenoids, and other pigments .However, Raman and absorption dynamics still is unclear [1,2] and here were present three main results for Raman study, Forbidden state modeling and complex search from Molecular Dynamics (MD)

We investigated LYC/β-CD complexes (Fig. 1) using MD and by comparing the results with experimental Raman data for LYC/HP-CD. We demonstrate that the Raman v_1 mode shifts to either lower or higher frequencies depending on lycopene's position within the β-CD.

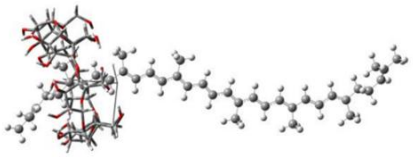

Fig. 1. Lycopene complex with β-cyclodextrin.

Using density functional theory (DFT), we calculate the structures and Raman spectra of various carotenoids and polyenes. We described energy diagrams of low-lying excited states with respect to Raman v_1 band using DFT and the ADC(n) family of correlated excited state methods (Fig. 2).

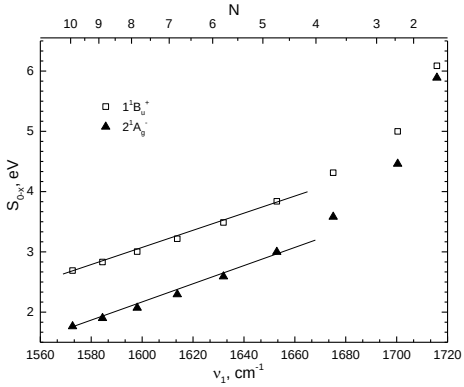

Fig. 2. Energy diagram for the low-lying singlet excited states of polyenes (N = 2–10).

MD calculations were performed on fucoxanthin in polar solvent by using methanol molecules. The properties of the lowest active excited states were evaluated. For this task QM/MM approach is established by using DFT methods. We find that the lowest optically allowed transition shifts to lower energies. New states with f>0.1 have not been identified.

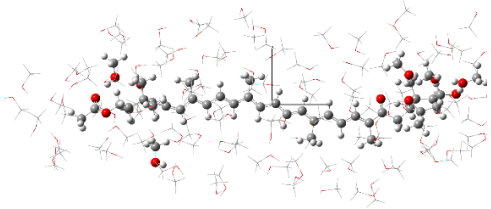

Fig. 3. Fucoxanthin QM/MM simulation

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