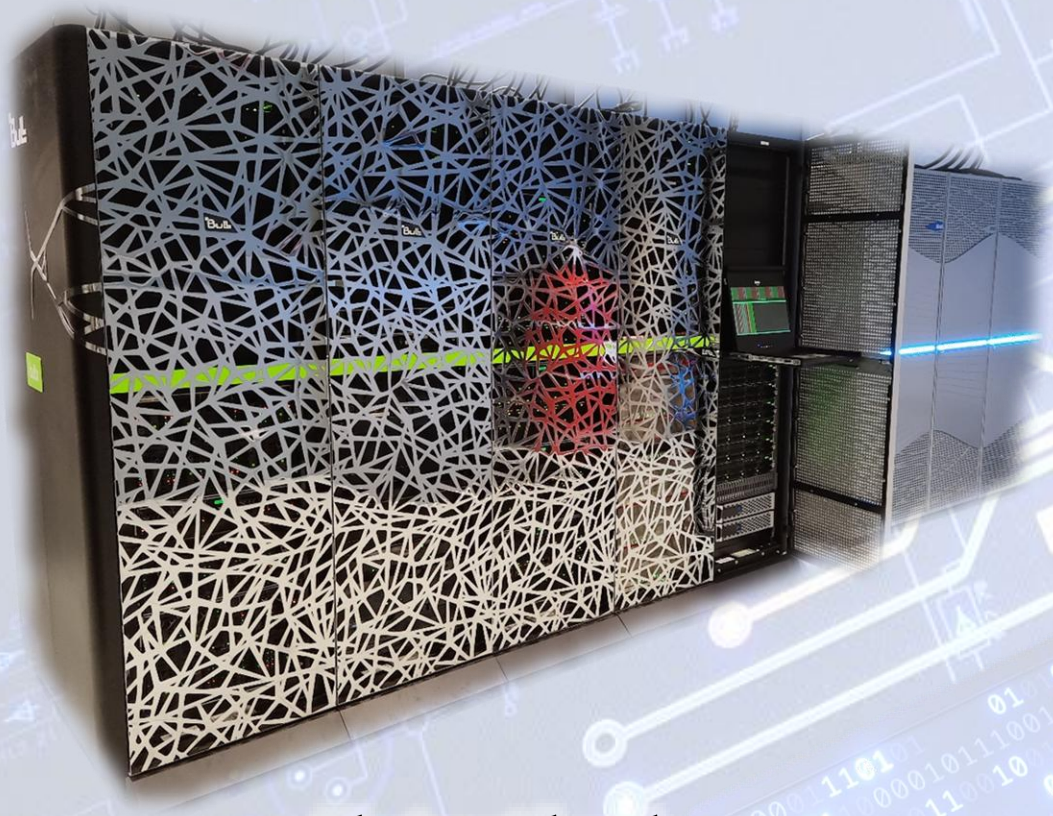
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Challenges in Modeling Molecular Aggregates Using HPC: Insights from Molecular Dynamics and Density Functional Theory

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Various molecular systems, including solvents, crystals, and protein aggregates, behave according to their initial conditions, as observed in carotenoids, stilbene, and Bis(diphenylphosphino)methane (dppm), Meso-tetra(4-sulfonatophenyl) porphine (TPPS4) [1-4]. Molecular Dynamics (MD) effectively captures solvent and protein dynamics, but its limitations become evident when describing processes transitioning from solvent to crystal. Here, systems are presented in which aggregated structural properties were successfully modeled using MD simulations.

Using MD simulations, we analyzed LYC/β-CD complexes (Fig. 1) and compared the results with experimental Raman data for LYC/HP-CD. We found that the Raman v1 mode exhibits frequency shifts, either lower or higher, based on the positioning of lycopene within the β-CD [1]. Notably, this reveals that β-CD enables the investigation of LYC as a monomer. However, the solid-state behavior of LYC remains an unresolved question.

TPPS4, a molecular nano-wire model, forms chiral nanotubes in acidic conditions, and our MD-based strategy identifies a probable zwitterionic tetramer structure responsible for large aggregate formation [3].

By combining Car-Parrinello Molecular Dynamics, big data analytics, and Density Functional Theory, we identified seven conformers with unique P-P through-space J-coupling properties in dppm[2].

MD simulations were conducted on fucoxanthin in a polar solvent using methanol molecules. The properties of the lowest active excited states were evaluated in various carotenoids (Fig 2.), and energy diagrams of low-lying excited states were described relative to the Raman v1 band using DFT and the ADC(n) family of correlated excited-state methods.

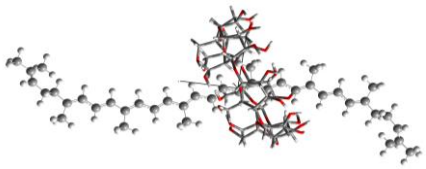

Fig. 1. Lycopene complex with β-cyclodextrin.

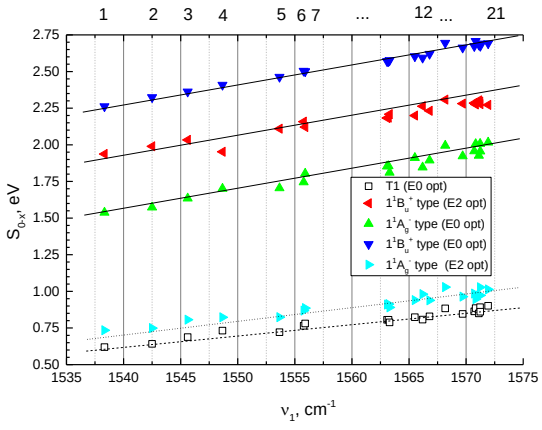

Fig. 2. States and correlation with Raman ν_1 for the various length Carotenoids.

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