Spectral and Molecular Dynamics Studies of Carotenoids and Stilbene in Complex Systems for Supercomputing

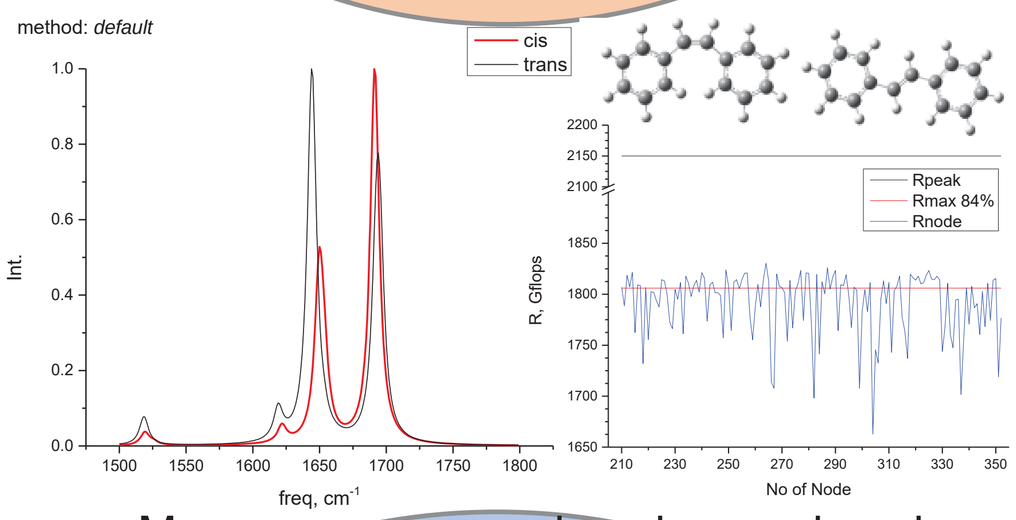
Mindaugas Mačernis, Goda Bankovskaitė, Jonas Franukevičius, Darius Abramavicius

Institute of Chemical Physics, Faculty of Physics, Vilnius University, Vilnius, Lithuania

E-mail: mindaugas.macernis@ff.vu.lt

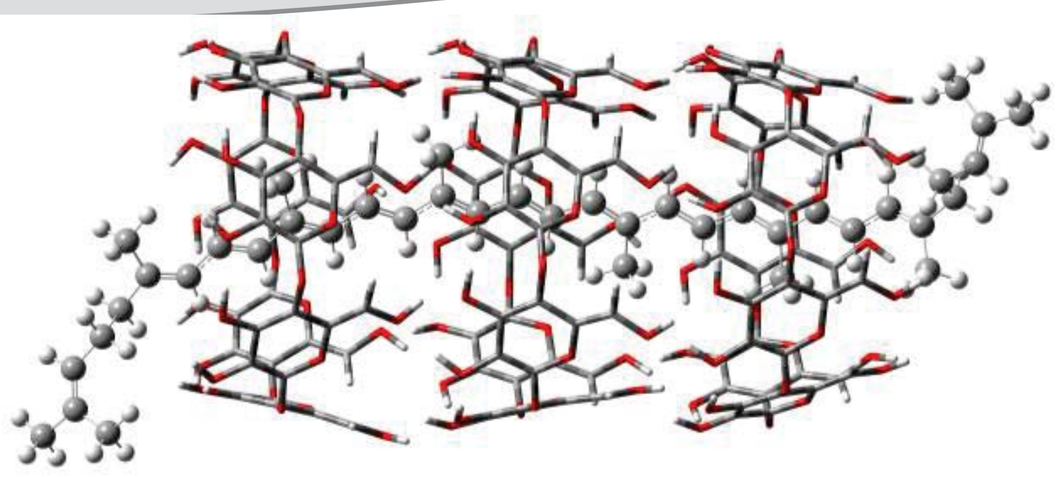
Molecular dynamics (MD) can utilize thousands of cores for research studies [1]. However, the Newtonian laws lack quantum physics phenomena, which are essential for understanding molecular properties in solvents, crystals, and amorphous materials [1-4]. Quantum MD methods, such as Car-Parrinello and Atom-Centered Density Matrix Propagation (ADMP) models or AIMD, can be updated to include excited-state dynamics, but understanding remains limited regarding physical properties and computational benchmarks [2-4]. In this study, we present results and discussions on the challenges of Quantum MD for selected carotenoids (Cars), stilbene, and other specific molecules in complex systems.

According to MD and DFT Raman analysis of lycopene and β-cyclodextrin interactions, we demonstrate that the Raman v1 mode shifts to lower or higher frequencies depending on the position of lycopene within the β-cyclodextrin. While MD provides insights into possible structural properties, it remains sensitive to the chosen environment, making it challenging to accurately model the complex dynamics of the lycopene and β-cyclodextrin system. Separate classical and quantum analyses are required.



Moreover, phosphorus-phosphorus through-space indirect spin-spin J-couplings in different conformations, as derived from QMD, present challenges for conformer identification (Fig. 1). Using our proposed Molecular Dynamics Conformation Probability analysis, we identified at least five distinct conformers in $CH(PPh_2)_2$.

In conclusion, we discuss the limitations of MD and QMD methods in larger-scale supercomputers.



Stilbene molecules are relatively small compared to carotenoids, but new methods are needed to interpret experimental data [4]. The combination of various Quantum MD approaches provides a deeper understanding, though it makes the required computational resources less predictable.

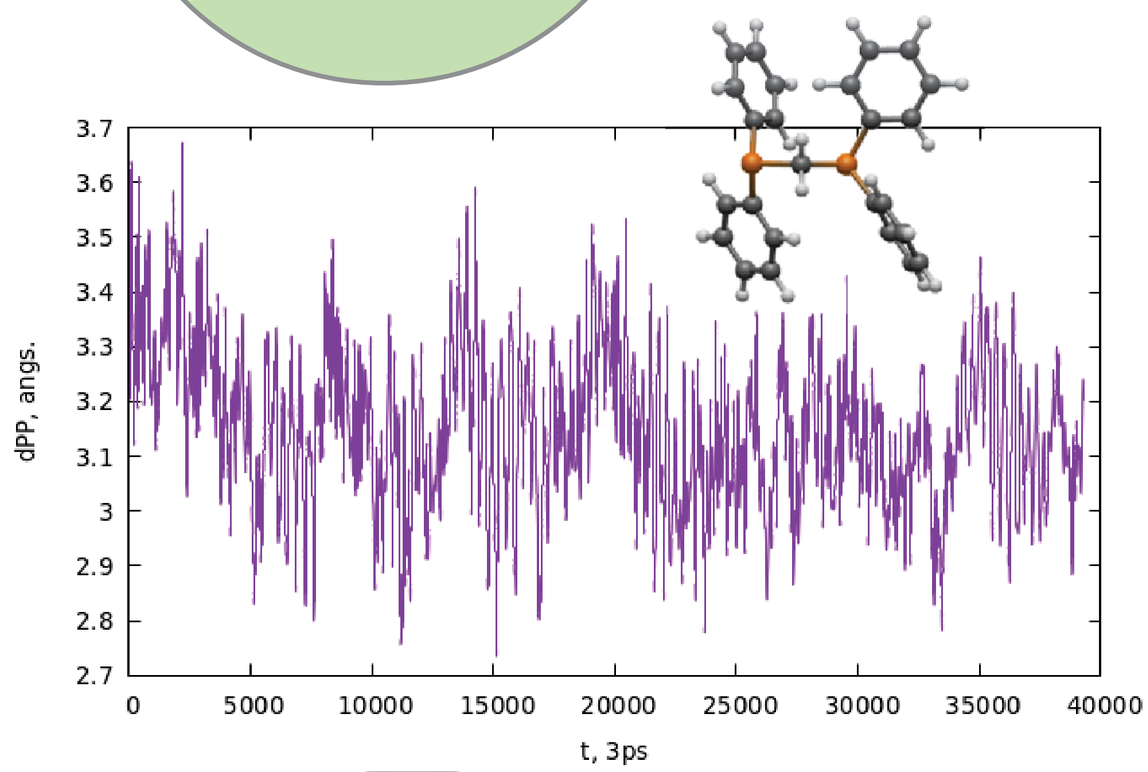


Fig. 1. The P-P distance from Quantum MD is crucial for understanding NMR-based quantum computing.

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