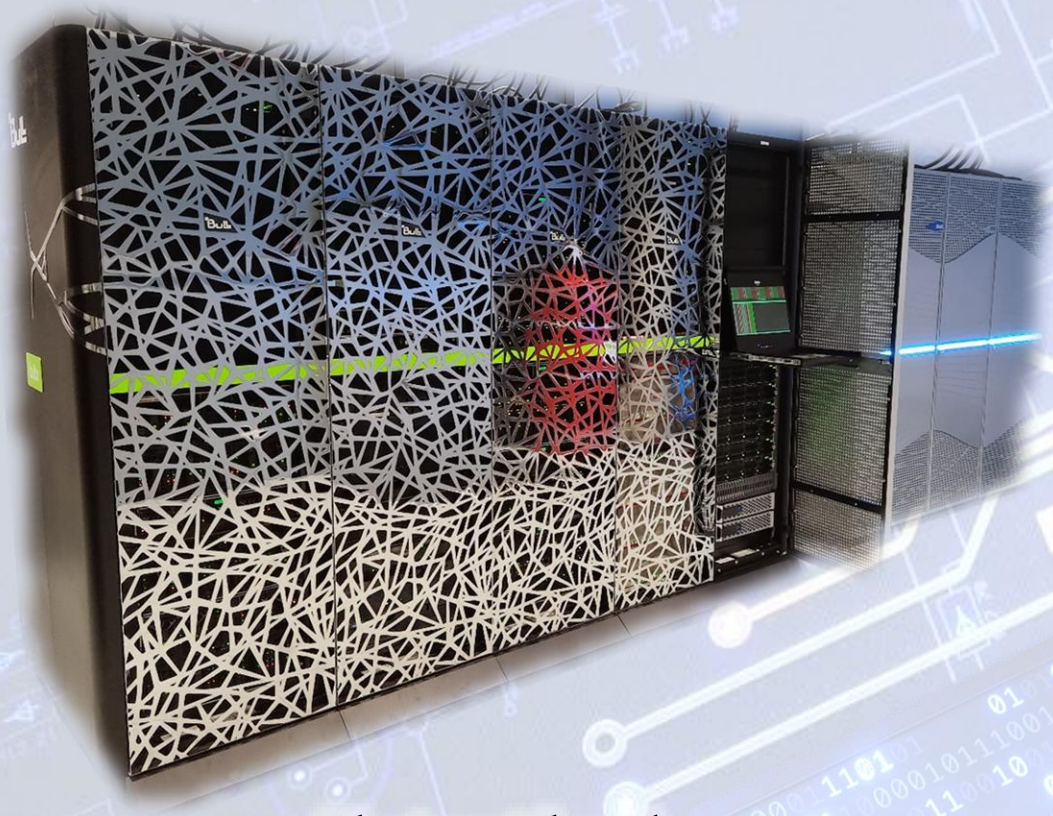
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Theoretical study of $TPPS_4$ aggregation

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Water-soluble, metal-free, highly stable aggregates are important as possible theranostic agents for photoacoustic imaging (PAI) and for photodynamic therapy (PDT) due to the intense light absorption in the phototherapeutic window. The 5,10,15,20-tetrakis(4-sulfonatophenyl) porphyrin ($TPPS_4$) molecules absorb light and initiate the activation processes leading to the death of the tumor cells, hence, could be used in PDT [1]. The monomers of $TPPS_4$ efficiently self-associate into large J-aggregates (side-by-side) or H-aggregates (face-to-face) in aqueous media depending on the concentration of $TPPS_4$ molecules and pH value of the solution. It is still not clear what type of aggregates are formed in specific conditions. Due to this reason we innvestigate how tetramers could formed.

The goal of this study is to determine the most stable zwitterionic $TPPS_4$ tetramers. QM geometry optimization of the zwitterionic TPPS4 Z1 and Z2 monomers was performed to determine molecular configuration using DFT B3LYP with Pople 6-311G(d,p) basis set. The Gaussian 16 C.01 program [2] was used. The next step was to take parameters from the GAFF. It was also adjusted several parameters of monomers. MM geometry optimization was also performed. Z1 and Z2 tetramers were constructed and solvated in box of water before MD simulation. MD simulation was also performed. In this research, the AMBER 22 [3] program was used.

We performed QM and MM optimizations of the $TPPS_4$ Z1 and Z2 monomers. The GAFF description of these monomers was revised. Two linear $TPPS_4$ Z1 and Z2 tetramers were constructed and their MD simulation was performed. The intermolecular curvature angle of these tetramers were calculated. It was determined that $TPPS_4$ Z1 and Z2 tetramers tend to curl into circle.

REFERENCES

[1] G. G. Parra, D. S. Correa, E. Silveira-Alves, L. M. Almeida, M. A. R. Souza, L. De Boni, L. Misoguti, C. R. Mendonça, S. C. Zílio, N. M. B. Neto, I. E. Borissevitch, P. J. Gonçalves, Effects of meso tetrakis (4-sulfonatophenyl) porphyrin (TPPS4) aggregation on its spectral and kinetic characteristics and singlet oxygen production, *Spectrochim Acta A Mol Biomol Spectrosc*. 261, 120063 (2021).

[2] M. J. Frisch, G. W. Trucks, H. B. Schlegel, …, D. J. Fox, Gaussian 16, Revision C.01, Gaussian, Inc., Wallingford CT (2016).

[3] D.A. Case, H.M. Aktulga, K. Belfon, ..., P.A. Kollman, Amber 2023, University of California, San Francisco (2023).