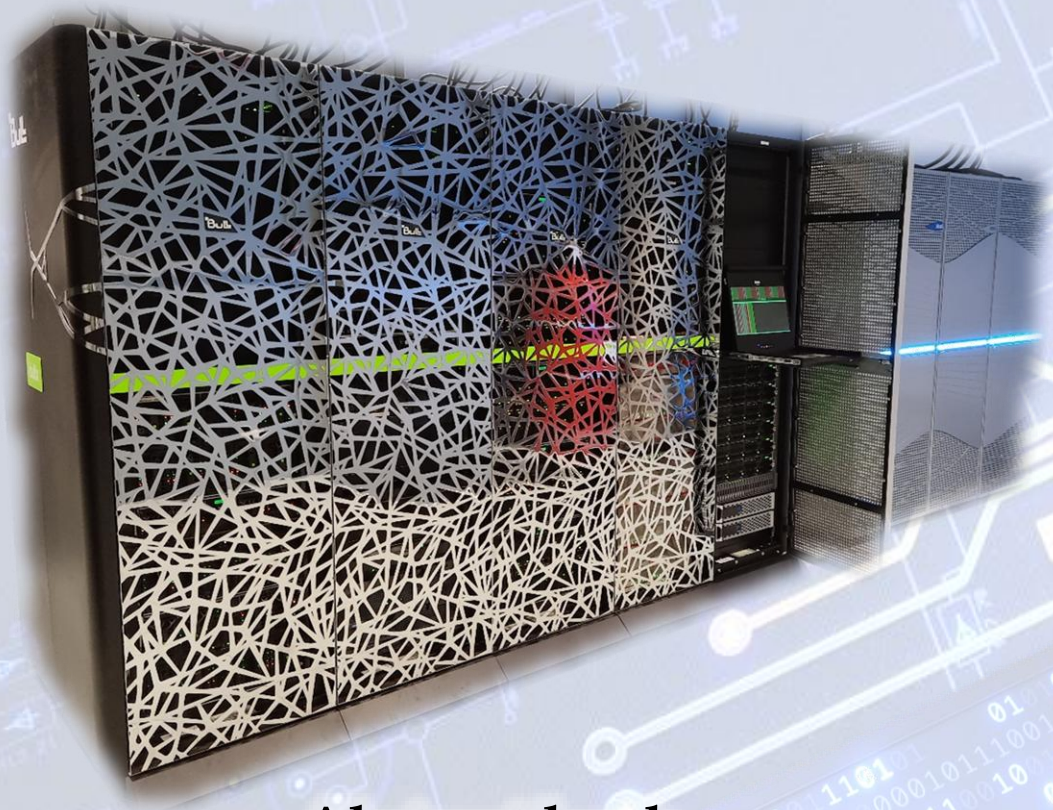
4TH EUROCC VILNIUS HACKATHON & WORKSHOP ON USING HPC



Abstract book

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Modeling of molecular nanotubes and their optical spectra

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Large organic molecular aggregates have promising applications as nonlinear optical elements, active materials in photodynamic therapy, and other photonic technologies [1]. In particular, the porphyrin TPPS4 forms two zwitterionic species (Z1 and Z2) at $pH = 1$, which self-assemble into molecular nanotubes that can exist in left-handed (M) or right-handed (P) forms, exhibiting notable optical properties [2]. Although the macroscopic structure of these nanotubes is well studied, their microscopic structure - including the molecular orientation - remains poorly understood. This study develops a theoretical model of these nanotubes and employs the Frenkel excitonic framework to optimize their microscopic arrangement by reproducing their linear optical spectra.

The nanotube is modeled by constructing a 2D crystal lattice with a constant of $a = 9.3$ Å, which is then rolled into a cylinder to form a tubular lattice of equally spaced points. A molecule is assigned to each point, each with four optical transition energies (two for the B band and two for the Q band), characterized by optical transition dipole vectors. Due to the molecule's planar symmetry, all dipole vectors lie within a defined molecular plane, whose orientation is described by a normal vector $\boldsymbol{n}$. Optical spectra are calculated by constructing the nanotube's Hamiltonian and solving the stationary Schrödinger equation to determine transition energies and wavefunctions. Optimization of the molecular plane's orientation is achieved by introducing two parameters, α_1 and α_2, which rotate the plane of each molecule relative to its lattice site.

By fitting simulated absorption spectra to experimental data, optimal values of $\alpha_1 = 32°$ and $\alpha_2 = 26°$ were obtained. In addition to absorption, circular dichroism (CD) spectra were calculated for both M and P-type nanotubes in the B band, yielding results that closely match experimental measurements. Furthermore, spectra of partially formed nanotubes were simulated, revealing the dynamic evolution of spectral peaks with increasing tube size and number of windings. To improve the model's accuracy, the effects of diagonal disorder were also incorporated into the spectral calculations.

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