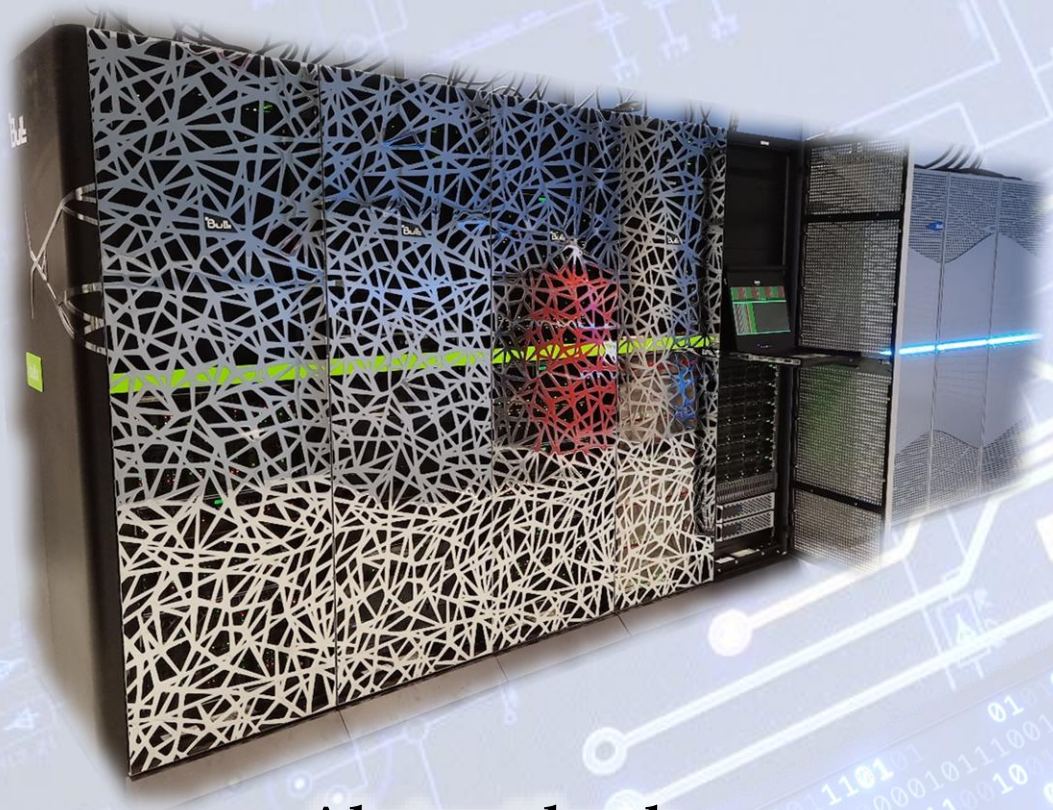
4TH EUROCC VILNIUS HACKATHON & WORKSHOP ON USING HPC



Abstract book

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Hackathon & Workshop organizers

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Structural Characterization of trans-Stilbene in Polystyrene Films via X-ray Diffraction

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The aggregation behavior of trans-stilbene in polymer matrices has recently attracted attention due to its impact on the optical and structural properties of hybrid organic materials. Previous studies have demonstrated that increasing the concentration of trans-stilbene in polystyrene (PS) films induces a transition from molecular dispersion to microcrystalline aggregation, significantly altering fluorescence lifetimes and spectral features [1], However, the crystallographic characteristics of these aggregates remain underexplored.

In this work, we present X-ray diffraction (XRD) measurements of thin films composed of polystyrene and trans-stilbene mixtures, prepared by solution casting onto zero-background substrates. The films were analyzed using a sealed 2 kW X-ray tube and a silicon strip detector in a θ–θ geometry. Diffraction patterns were recorded for various stilbene concentrations (5–80%, where 100% corresponds to a 1:1 mass ratio of stilbene to PS). The results reveal the emergence of distinct diffraction peaks at higher concentrations, consistent with the formation of microcrystalline domains previously observed via CARS and AFM microscopy [2].

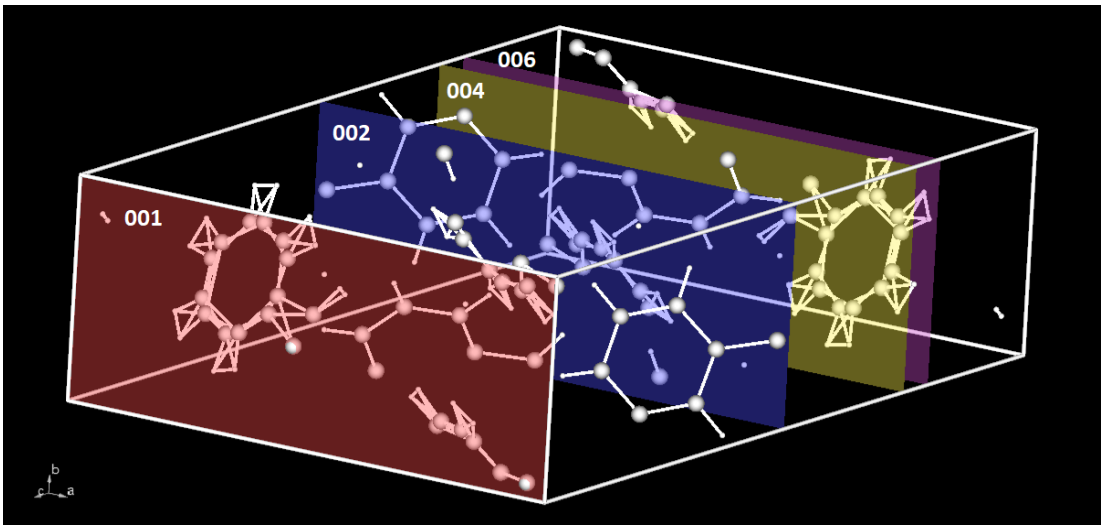

Fig. 1. Planes observed (001, 002, 004 and 006) of the pure stilbene depicted in primitive crystal lattice

REFERENCES

[1] I. Halimski *et al.*, “trans -Stilbene aggregates and crystallites in polystyrene films: microscopy and spectroscopy studies,” *Phys. Chem. Chem. Phys.*, vol. 26, no. 36, pp. 23692–23702, 2024, doi: 10.1039/D4CP02291B.

[2] R. Karpicz, G. Kareivaite, M. Macernis, D. Abramavicius, and L. Valkunas, “Two phases of *trans* -stilbene in a polystyrene matrix,” *Phys. Chem. Chem. Phys.*, vol. 25, no. 32, pp. 21183–21190, 2023, doi: 10.1039/D3CP03015F.