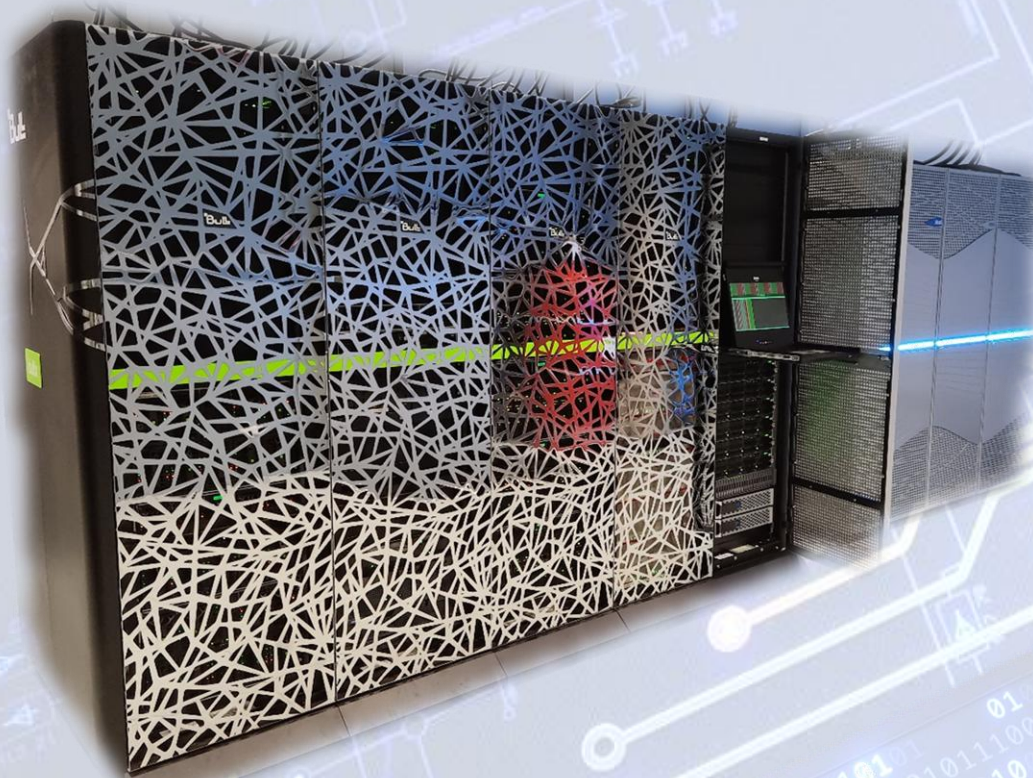




4TH EUROCC VILNIUS HACKATHON & WORKSHOP ON USING HPC



Abstract book

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Hackathon & Workshop organizers

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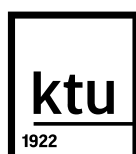
Project Implementers



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Quantum-chemical exploration of the methanol-sensing mechanism of the *meso*-formyl BODIPY compounds

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Molecular compounds based on the boron-dipyrromethene (BODIPY) group have been shown to have promising potential for use as microscopic, single-molecule optical (fluorescence lifetime-based) sensors of environment properties, such as temperature or viscosity. The compounds exhibit complex energy-relaxation behavior depending on the surroundings, which necessitates both experimental and theoretical research of their own properties [1].

A recent study conjectured how a *meso*-formyl BODIPY derivative (Fig. 1) could act as an optical sensor for cellular viscosity and methanol concentration in the molecule's vicinity. However, an attempt to increase the fluorescence wavelength for better compatibility with biological samples (by changing the molecular structure) resulted in the loss of both polarity and viscosity sensitivity [2].

In this work, a theoretical investigation of the excitation-induced processes of *meso*-formyl BODIPY variants in methanol [3] is continued, assessing the experimental claims and trying to answer questions like: how a non-emissive molecule is a fluorescence-lifetime target? how would it benefit from a reaction with textbook barrier energy comparable to that of the optical excitation? ...and others.

The research is supported by the Research Council of Lithuania (LMT grant no. S-MIP-23-48). Quantum-chemical computations were performed using resources at the supercomputer "VU HPC" of Vilnius University in the Faculty of Physics location [4].

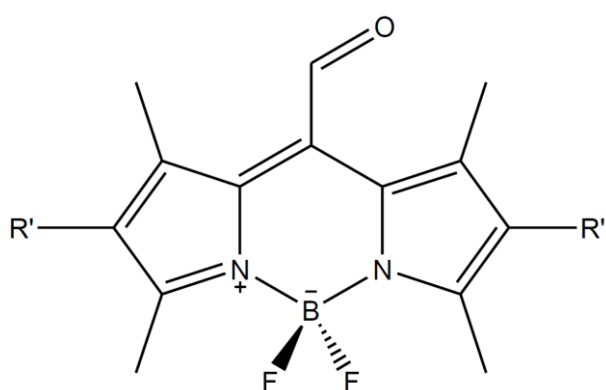


Fig. 1. Chemical structure of *meso*-formyl BODIPY derivatives.

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- [4] Supercomputer "VU HPC" Saulėtekis. [Online: <https://sauletekis.ff.vu.lt/en/>]