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Analysing Bulk- and Microviscosity Effects from Multi-Level Computation Results of the Properties of BODIPY-Based Molecular Sensors

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Molecular compounds based on boron-dipyrromethene (BODIPY) have been shown to be promising candidates for microscopic, single-molecule scale sensing of environment properties, such as viscosity or temperature [1]. It is also possible to anchor the sensors to a specific type of microscopic environment, e.g., a lipid cell membrane, where the restricted molecular drift and its fluctuations result in a measurable estimate of the bulk viscosity and temperature, respectively [2]. This work builds upon an existing quantum-chemical model of microviscosity sensitivity applied to the snapshots of molecular dynamics simulations of a BODIPY sensor anchored in a bilayer lipid membrane [3]. Intensity and timescales of the dynamic changes in expected microviscosity sensitivity are evaluated by analysis of the results of the computations of the molecular properties with the aim to determine how much the bulk drift (spanning 2-12 ns) influences the fluorescence lifetime-based viscosity measurements of the sensors (0,1-5 ns). Quantum-chemical computations and subsequent data analysis were performed using resources at the supercomputer "VU HPC" of Vilnius University in the Faculty of Physics location.

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