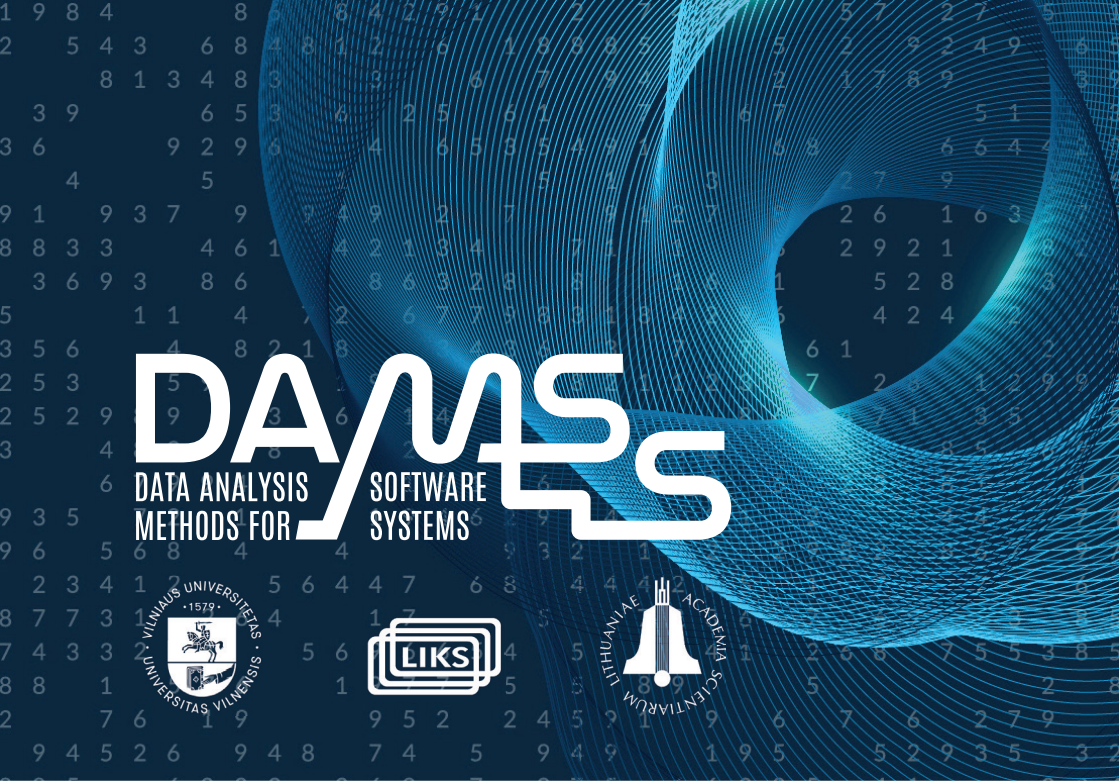


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# Looking for Simplified Molecular Reaction Coordinates from Computation Data

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A range of molecular sensors for measuring properties in micro-scopic environments is based on BODIPY (boron-dipyrromethene) molecule with a rotation-capable chemical group attached. The sensing mechanism can be modeled, as a first approximation, by the evolution of the electronic excitation along the potential-energy curve of the lowest excited state with respect to the rotation angle. However, the nontrivial structure of base and rotation groups presents several challenges for such an approximation.

A reaction coordinate based on the average of opposite dihedral angles, as applied in [1] and later works, is shown to better estimate the actual rotation than a single rotation angle, both for symmetric and asymmetric rotation groups. A similar approach is currently being studied to estimate the mean curvature in TPPS4 (meso-tetra-(4-sulfonatophenyl) porphyrin) oligomers.

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[1] Toliautas, S., Dodonova, J., Žvirblis, A., Čiplys, I., Polita, A., Devižis, A., Tumkevičius, S., Šulskus, J., Vyšniauskas, A., Enhancing the Viscosity-Sensitive Range of a BODIPY Molecular Rotor by Two Orders of Magnitude. Chemistry – A European Journal, vol. 25, 2019, pp. 10342-10349.