Exploring the influence of electron donor and acceptor substituents on photochemical properties of a light-driven molecular nanomotor

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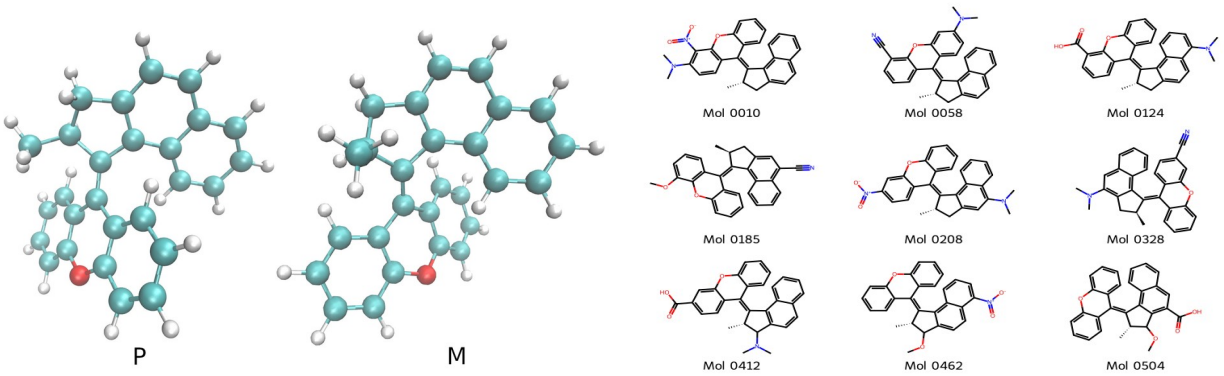

We report an analysis of the impact of the molecular structure on the photochemical excited state properties of a comprehensive dataset of 2016 compounds based on the structure of a second-generation light-driven molecular nanomotor. [1,2] The two main helical conformers of the base structure were modified with all combinations of one electron donor and one acceptor group from a pool of three each on eight possible positions. We performed ground state geometry optimizations and excited-state calculations using time-dependent density functional theory to obtain the excitation energies, oscillator strengths and two photon absorption strengths of the first two excited states. [3] To identify the reactive state, transition densities were calculated and compared with the unsubstituted nanomotors. Further, a benchmark study of three machine learning models and three molecular descriptors was performed to accelerate the identification of promising candidates for future applications in living tissue without the need for expensive quantum mechanical calculations.

[1] V. García-López, F. Chen, L. Nilewski, et al, *Nature,* **2017**, *548*, 567–572.
[2] B. Oruganti, C. Fang, B. Durbeej, *Phys. Chem. Chem. Phys.*, **2015**, *17*, 21740-21751.
[3] R. Ramakrishnan, M. Hartmann, E. Tapavicza, et al, *J. Chem. Phys.*, **2015**, *143* (*8*), 084111