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Photoisomerization dynamics of a rhodopsin-based molecule (potential molecular switch) with high quantum yields[1] ROLAND ALLEN, Texas A&M University, CHEN-WEI JIANG, Xi'an Jiaotong University, XIU-XING ZHANG, Weinan Normal University, AI-PING FANG, HONG-RONG LI, RUI-HUA XIE, FU-LI LI, Xi'an Jiaotong University — It is worthwhile to explore the detailed reaction dynamics of various candidates for molecular switches, in order to understand, e.g., the differences in quantum yields and switching times. Here we report density-functional-based simulations for the rhodopsin-based molecule 4-[4-Methylbenzylidene]-5-p-tolyl-3,4-dihydro-2H-pyrrole (MDP), synthesized by Sampedro et al. We find that the photoisomerization quantum yields are remarkably high: 82% for *cis*-to-*trans*, and 68% for *trans*-to-*cis*. The lifetimes of the S_1 excited state in *cis*-MDP in our calculations are in the range of 900-1800 fs, with a mean value of 1270 fs, while the range of times required for full *cis*-to-*trans* isomerization are 1100-2000 fs, with a mean value of 1530 fs. In *trans*-MDP, the calculated S_1 excited state lifetimes are 860-2140 fs, with a mean value of 1330 fs, and with the full *trans*-to-*cis* isomerization completed about 200 fs later. In both cases, the dominant reaction mechanism is rotation around the central C=C bond (connected to the pyrroline ring), and de-excitation occurs at an avoided crossing between the ground state and the lowest singlet state, near the midpoint of the rotational pathway.

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