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Dynamics of the photoisomerization process of *trans* - azobenzene: a time-dependent density functional study NORIHISA OYAMA, NIMS, YOSHITAKA TATEYAMA, NIMS, YOSHIYUKI MIYAMOTO, NEC, TAKAHISA OHNO, NIMS — Azobenzene is a typical molecule which shows a reversible photoisomerization, and has attractive considerable attention for molecular devices. The photoisomerization mechanism of *trans* - azobenzene, however, has been controversial for over a half century because of its ultra-fast reaction. In this work, we investigated the dynamics of the photoisomerization process of *trans*- azobenzene based on time-dependent density functional theory. Our calculations clearly indicate that the photoisomerization process for S_1 excitation occurs through a rotation channel against the widely-accepted inversion mechanism. In contrast, it was found that a direct isomeriza- tion does not occur for S_2 excitation, and a transition to S_1 occurs at about 100fs. This study was supported by ACT- JST, and FSIS and Special Coordination Funds of MEXT of the Japanese government. The calculations in this work were carried out partly using the Numerical Materials Simulator in National Institute for Materials Science, and partly using the NEC-SX5 at Cybermedia Center, Osaka University.

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