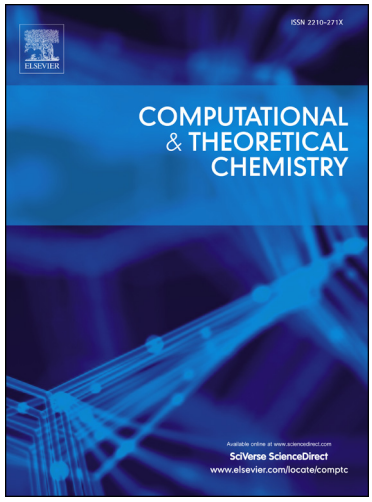

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Photochemical dynamics simulations for trans-cis photoisomerizations of azobenzene and bridged azobenzene

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Abstract

Surface hopping dynamics simulations based on the Zhu-Nakamura theory were performed to investigate the trans-cis photoisomerization mechanisms of azobenzene and bridged azobenzene excited to S_1 state. In geometry optimization, both for the two compounds, two minimum-energy conical intersections between the ground state and the lowest excited state are located. Two conical intersections are confirmed to be decay funnels in the trans-cis photoisomerization processes in azobenzene but only one plays important parts in the photoisomerization of bridged azobenzene. Due to the smaller slope of potential energy surface in the S_1 state, the lifetime of the S_1 state of azobenzene in our work is much longer than that of bridged azobenzene. We show that the torsion around the central N=N bond is the preferred reaction mechanism in the isomerization of two molecules. Rotation around the central N=N bond and twisting of phenyl rings around their N-C bonds allows the molecule to move to a minimum-energy conical intersection, after which surface hopping from S_1 to S_0 occurs. In the ground state, further rotation