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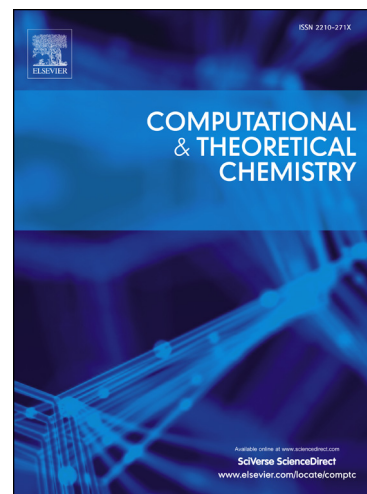
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1 Photochemical dynamics simulations for trans-cis photoisomerizations of
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9 **Abstract**

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

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