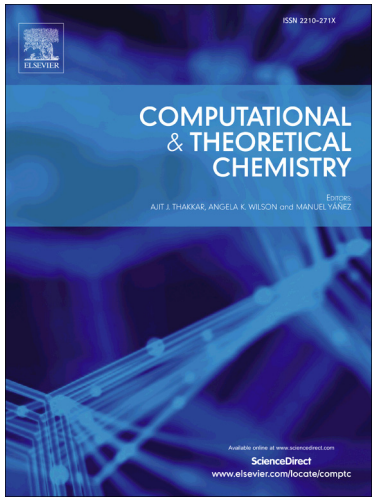

Substituent effect on the transport properties of dihydroazulene -based molecular optical switch: a way to tune the switching properties

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Substituent effect on the transport properties of dihydroazulene -based molecular optical switch: a way to tune the switching properties

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Abstract. The transport properties of dihydroazulene-based molecular optical switch were investigated by using first-principle calculation combined with non-equilibrium Green's function method. According to the results, the switch behavior is caused by the different localization of the frontier molecular orbitals of the isomers near the Fermi level. The effects of some substituents of Br, CH_3 and OH on the transport properties of this molecular optical switch were also studied. Theoretical results indicate that the switch behavior of such molecular device is determined mainly by the position of the substituents. These results provide a detailed physical picture and a way to manipulate

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