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QMC Study of Optical Switching of Azobenzene Molecule[1] RENE DERIAN, MATUS DUBECKY, Inst. of Phys., Slovak Academy of Sciences, Bratislava, Slovakia , LUBOS MITAS, Dept. of Phys., NCSU, Raleigh, IVAN STICH, Inst. of Phys., Slovak Academy of Sciences, Bratislava, Slovakia — Optical Switching of photochromic azobenzene (AB) molecule via first excited singlet-state is studied. AB features two photoswitchable conformations, cis and trans with very different geometries and properties. Using QMC techniques we compute excitation/deexcitation ground-state – first singlet- excited-state spectra of AB. By a careful QMC optimization of the ground/excited-state wave functions with up to 500 determinants chemical accuracy is obtained for the cis and trans conformers. Our QMC results are significantly superior to DFT results with proper spin symmetry (ROKS) and surpass also the available standard quantum chemistry results such as CAS SCF. These results open up the possibility of simulation of anchored AB opto-mechanical switches.

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