Abstract Submitted
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Electronic structure of azobenzene: ground and first excited singlet states[1] MATUS DUBECKY, RENE DERIAN, Inst. Phys., Slovak Acad. Sci, LUBOS MITAS, North Carolina State University, IVAN STICH, Inst. Phys., Slovak Acad. Sci — QMC techniques are used to obtain energies at selected points on the potential energy surfaces of a photoswitchable molecule, azobenzene (AB), along the torsion pathway (CNNC dihedral angle), in the ground and first excited singlet states. We study the excitation energies of well separable cis- and trans-conformers, and th Inst. Phys., Slovak Acad. Scie energy of the transition state located at 90°. By a careful QMC optimization of the Slater-Jastrow wavefunctions with up to 500 determinants, chemical accuracy is obtained. Our results not only outperform all the available quantum chemistry results such as CAS-SCF, CAS-PT2, as well as DFT results with proper spin symmetry taken into account (ROKS), but open also a credible window to possible correction/reinterpretation of the available experimental data.

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