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Rational Design of Two-Photon Absorbing Photochromic Materials for Optical Switching and Data Storage[1] I.A. MIKHAILOV, K.D. BELFIELD, A.E. MASUNOV, University of Central Florida — Diarylethenes are able to undergo light-induced transition from the open to closed ring isomer (photocyclization) accompanied by the change in optical properties (photochromism). This ability holds a great promise for photonic applications, including optical data storage and ultrafast optical switching. Photocyclization initiated by absorption of two photons could drastically increase the density of these devices. However, attachment of fluorene substituent to diarylethene to increase two-photon absorbing cross-section led to the loss of photochromic activity. Analysis of the Kohn-Sham orbitals reveals that the relaxation of the lowest excited state of diarylethene fragment leads to photocyclization, while the occupied level of the chromophore substituent generates an excited state below the photoreactive one. To design the molecular switch active in two-photon regime we suggest stabilizing the highest occupied orbital, which can be accomplished by fluorination of the chromophore. We applied time dependent Density Functional Theory to predict potential energy surfaces of excited states and two-photon absorbing profiles. The obtained results are in agreement with the qualitative orbital description.

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