Revealing the switching mechanisms of an OFF-ON-OFF fluorescent logic gate system

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Figure S1. $^1$H-NMR spectrum of M3.

Figure S2. Possible four protonated positions of M1-1H and relative Gibbs free energy of the corresponding protonated products (with two protons). Site II shows the highest reactive activation towards protonation (forming M1-2H).
Figure S3. Distribution of hole and electron in M1 and M1-1H. Green donates hole and pink for electron; D is the centroid distance of hole and electron; $S_r$ is overlap between hole and electron; $t$ index is designed to measure the degree of hole and electron separation in the charge transfer direction. If $t < 0$, hole and electron is not complete separated, and a more negative value of $t$ indicates a smaller degree of charge transfer.  

Figure S4. Distribution of molecular frontier orbitals, electronic transitions, and hole-electron analysis (a) before the protonation of M3 and (b) after the protonation of M3. Green donates hole and pink for electron; D is the centroid distance of hole and electron; $S_r$ is overlap between hole and electron; $t$ index
is designed to measure the degree of hole and electron separation in the charge transfer direction.

Figure S5. Potential energy surface (pink) of M3 in the S1 state and corresponding oscillator strength (blue) in acetonitrile, calculated using M062X.

Figure S6. Potential energy surface (pink) and corresponding oscillator strength (blue) of M1 in the S1 state in acetonitrile, calculated using CAM-B3LYP (a) and ωB97XD (b) functionals.

Figure S7. Potential energy surface (pink) and corresponding oscillator strength (blue) of M1 (a) and M3 (b) in the S1 state in water, calculated using M062X functional.
Figure S8. Relative potential energy surface (pink) of M1-1H in the S1 state in acetonitrile, calculated using M062X in combination with liner solvation model.

Figure S9. UV—vis absorption spectra of M3 in methanol and glycerol ([M3] = 10 μM).

Figure S10. Normalized UV-vis absorption spectra of M3 upon titration with 0 – 5 eq. of CF₃COOH in methanol.
Figure S11. Molecular frontier orbitals and electronic transitions of M2 in acetonitrile.

Reference