Electronic Supplementary Material (ESI) for Chemical Science.

Computational design of a molecular triple photoswitch for wavelength-selective control

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Supporting Information

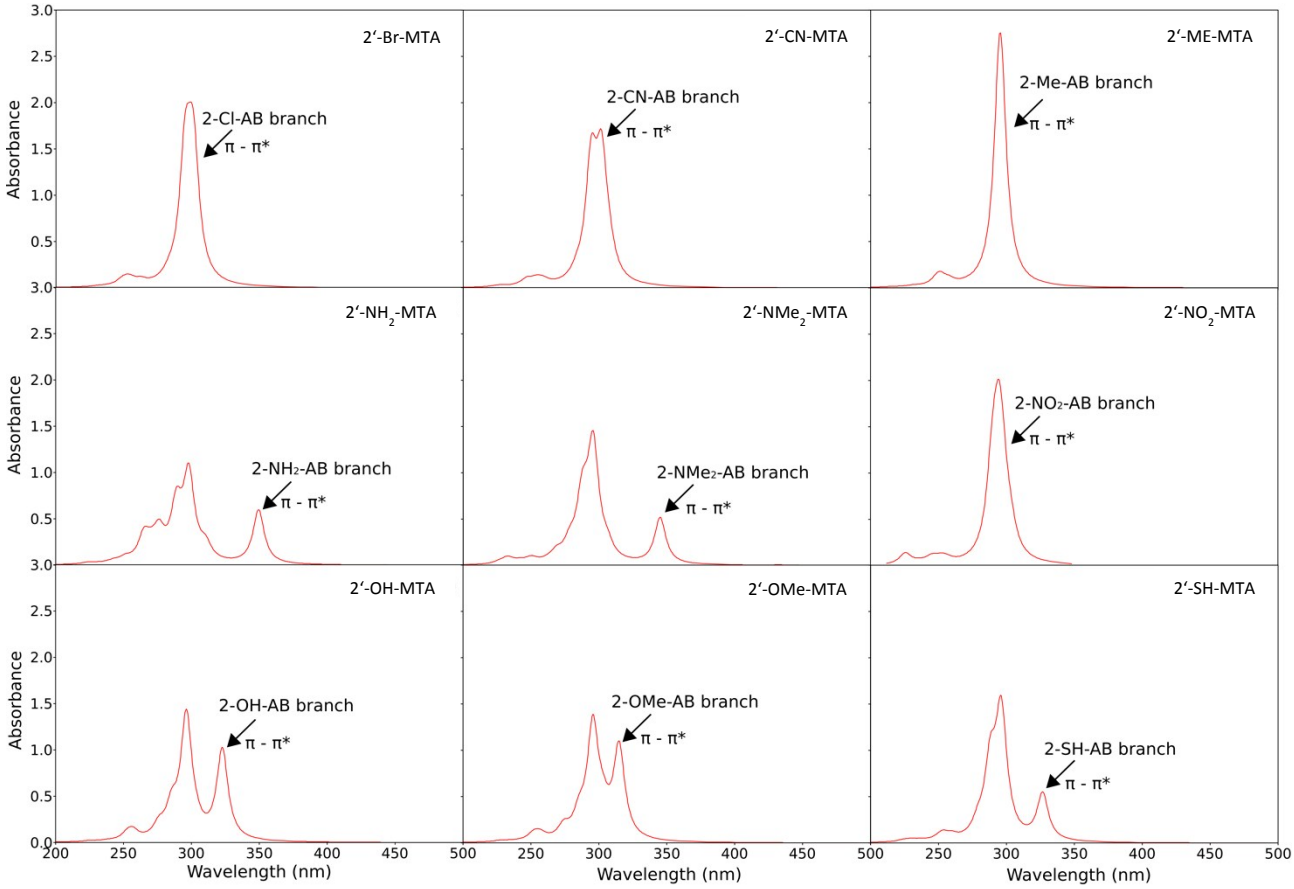

Figure S1: Simulated absorption spectra of single-branch substituted MTAs, which are all substituted at the 2' position, at the theoretical level of TDDFT/CAM-B3LYP. For the simulation of the spectra a full-width-at-half maximum of 10 nm has been used.

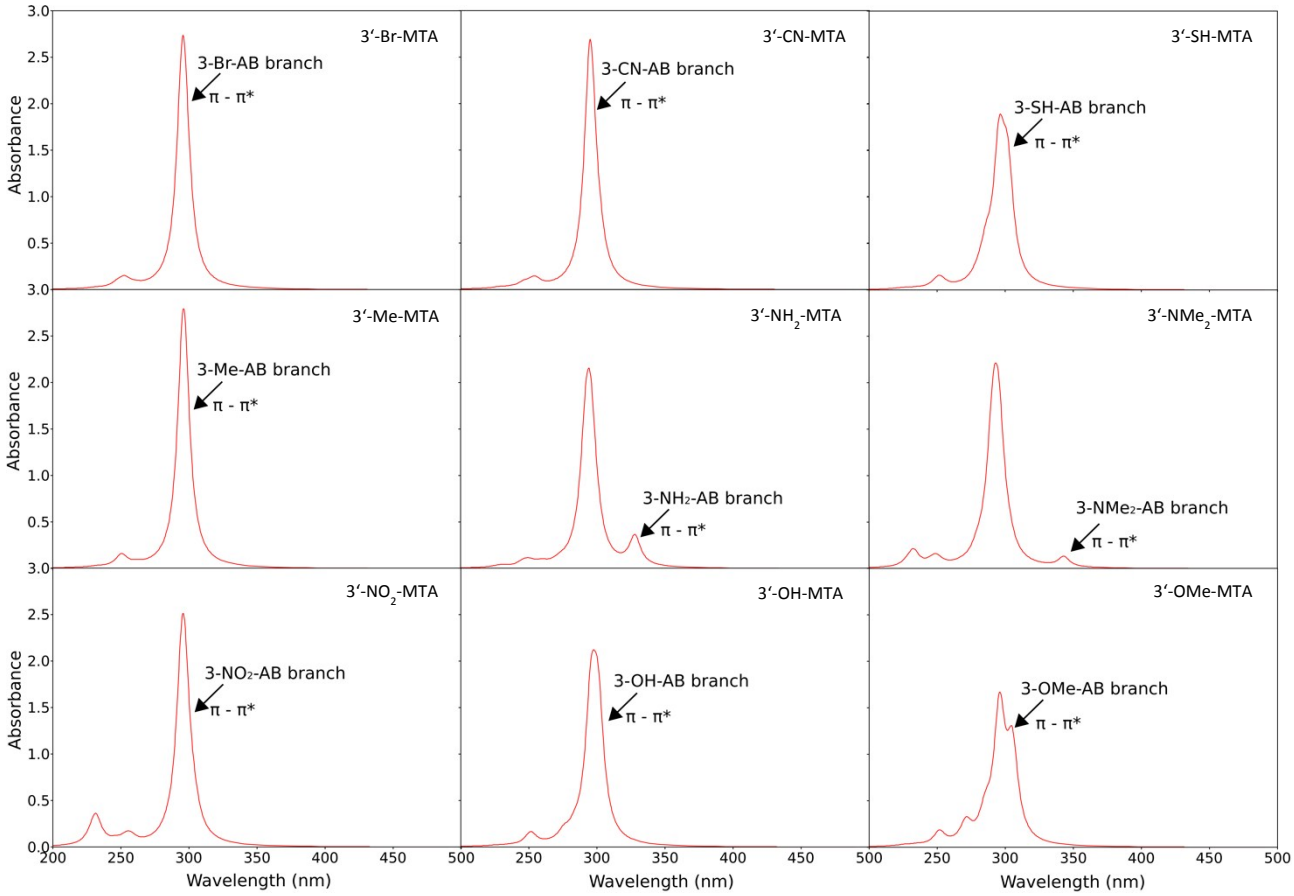

Figure S2: Simulated absorption spectra of single-branch substituted MTAs, which are all substituted at the 3' position, at the theoretical level of TDDFT/CAM-B3LYP. For the simulation of the spectra a full-width-at-half maximum of 10 nm has been used.

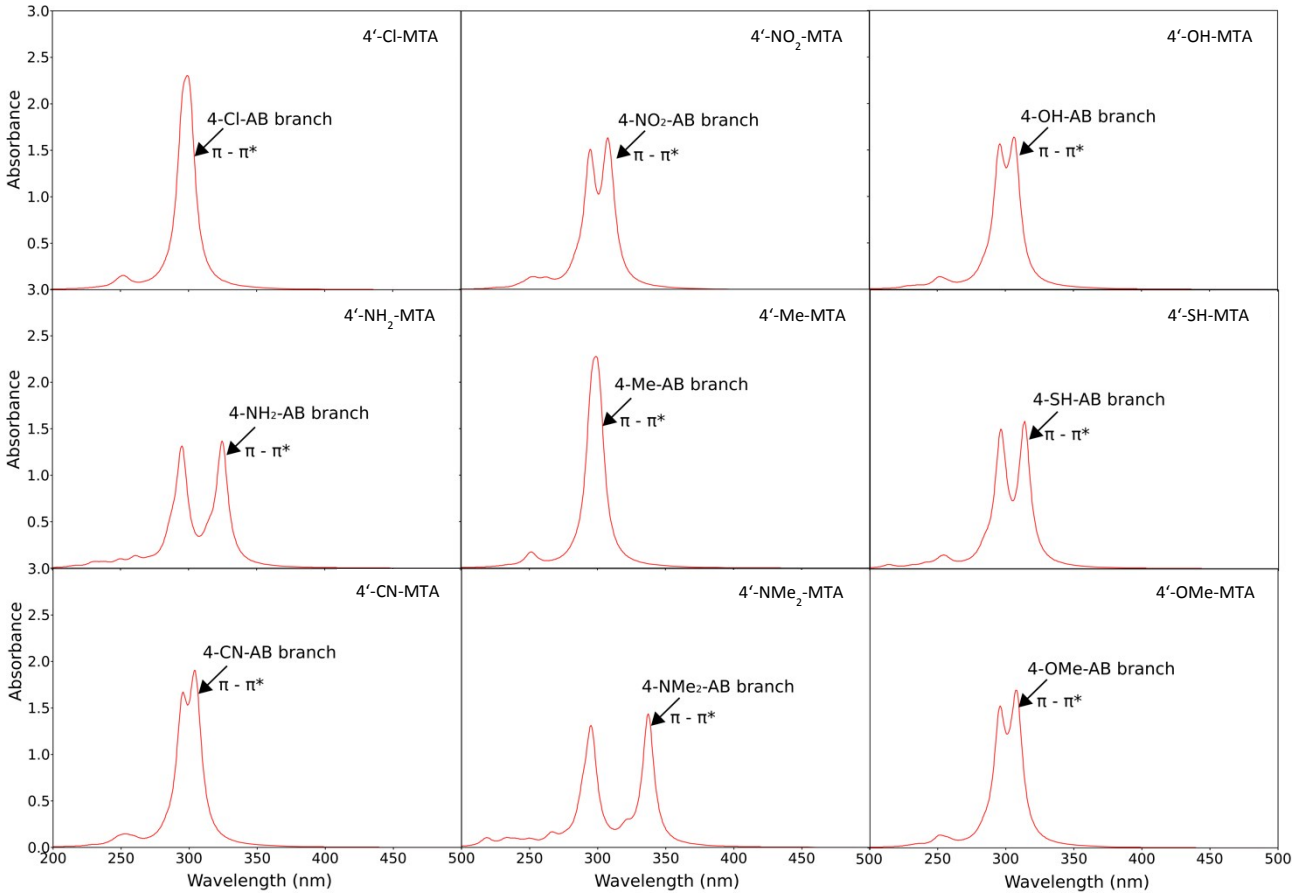

Figure S3: Simulated absorption spectra of single-branch substituted MTAs, which are all substituted at the 4' position, at the theoretical level of TDDFT/CAM-B3LYP. For the simulation of the spectra a full-width-at-half maximum of 10 nm has been used.

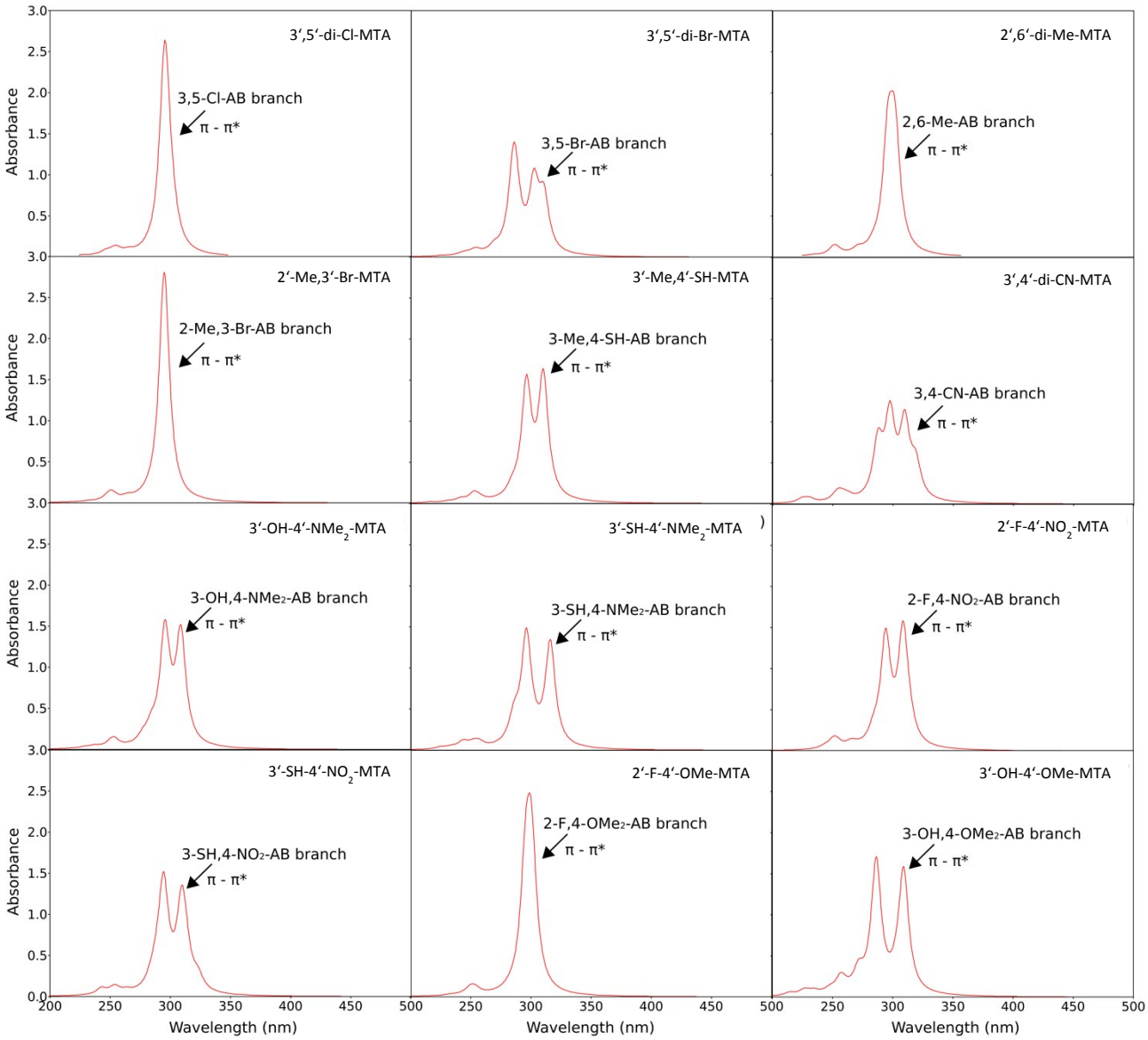

Figure S4: Simulated absorption spectra of single-branch substituted MTAs with two substituents at one terminal phenyl ring at the theoretical level of TDDFT/CAM-B3LYP. For the simulation of the spectra a full-width-at-half maximum of 10 nm has been used.

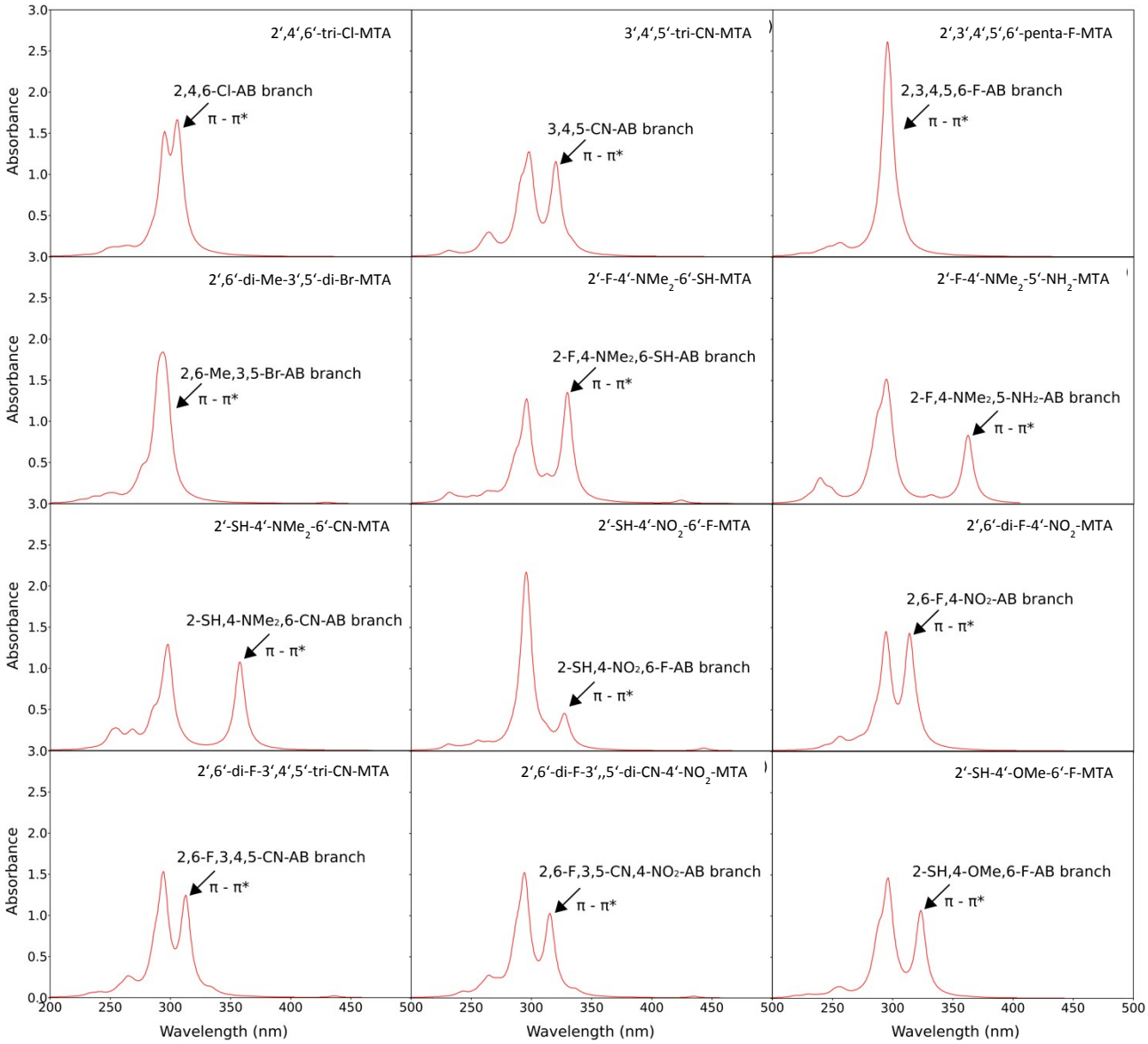

Figure S5: Simulated absorption spectra of single-branch substituted MTAs with multiple substituents at one terminal phenyl ring at the theoretical level of TDDFT/CAM-B3LYP. For the simulation of the spectra a full-width-at-half maximum of 10 nm has been used.

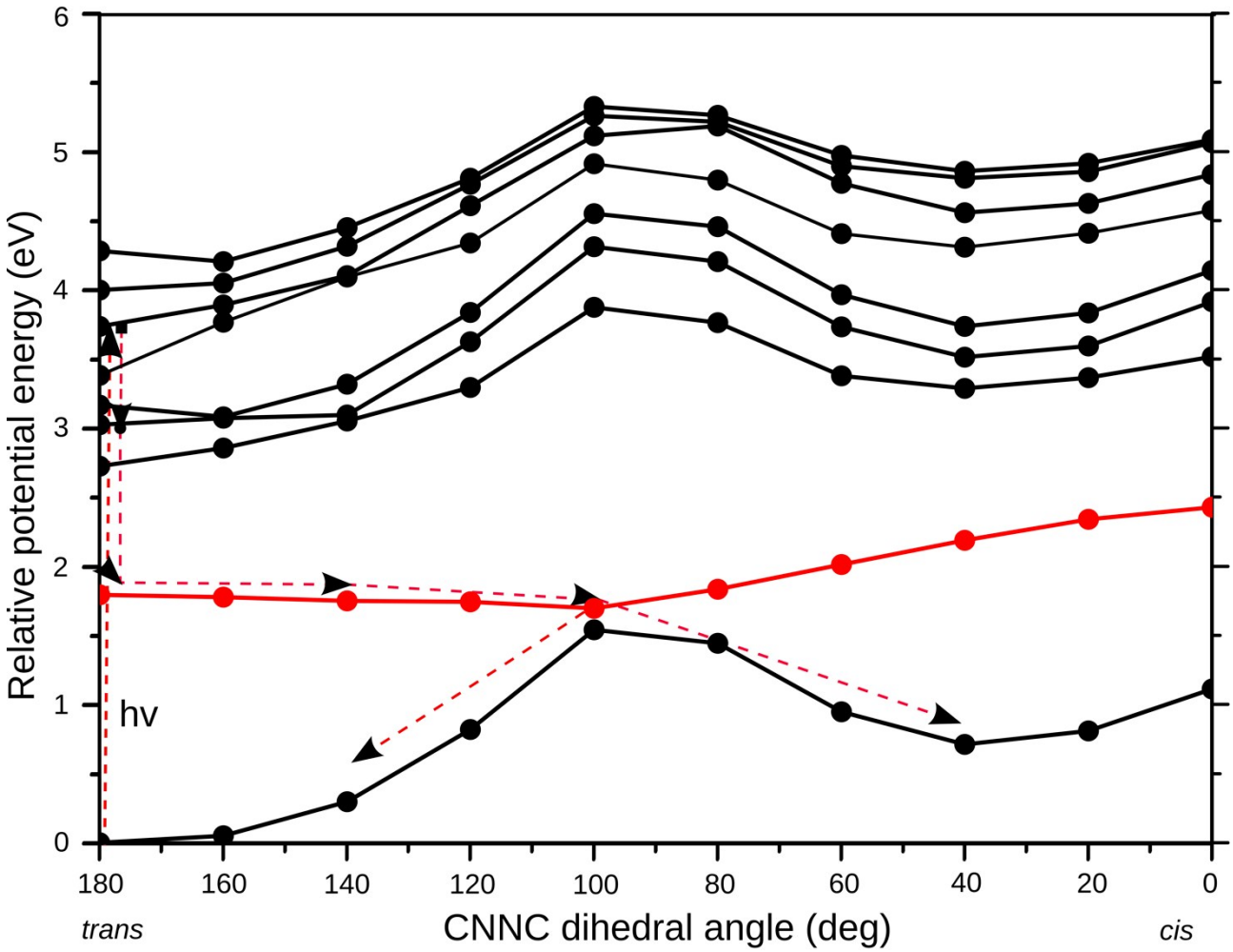

Figure S6: Relaxed scans of the potential energy surfaces along the isomerization pathway of the 4''-SH substituted AB branch of (2',4',6'-tri-CN-4''-SH)-MTA after unconstrained relaxation of S_6. Initially, the excited S_6 $\pi\pi^*$ state decays into the S_1 $n\pi^*$ now localized at the 4''-SH substituted AB branch, which undergoes barrierless isomerization along the CNNC dihedral angle rotation.

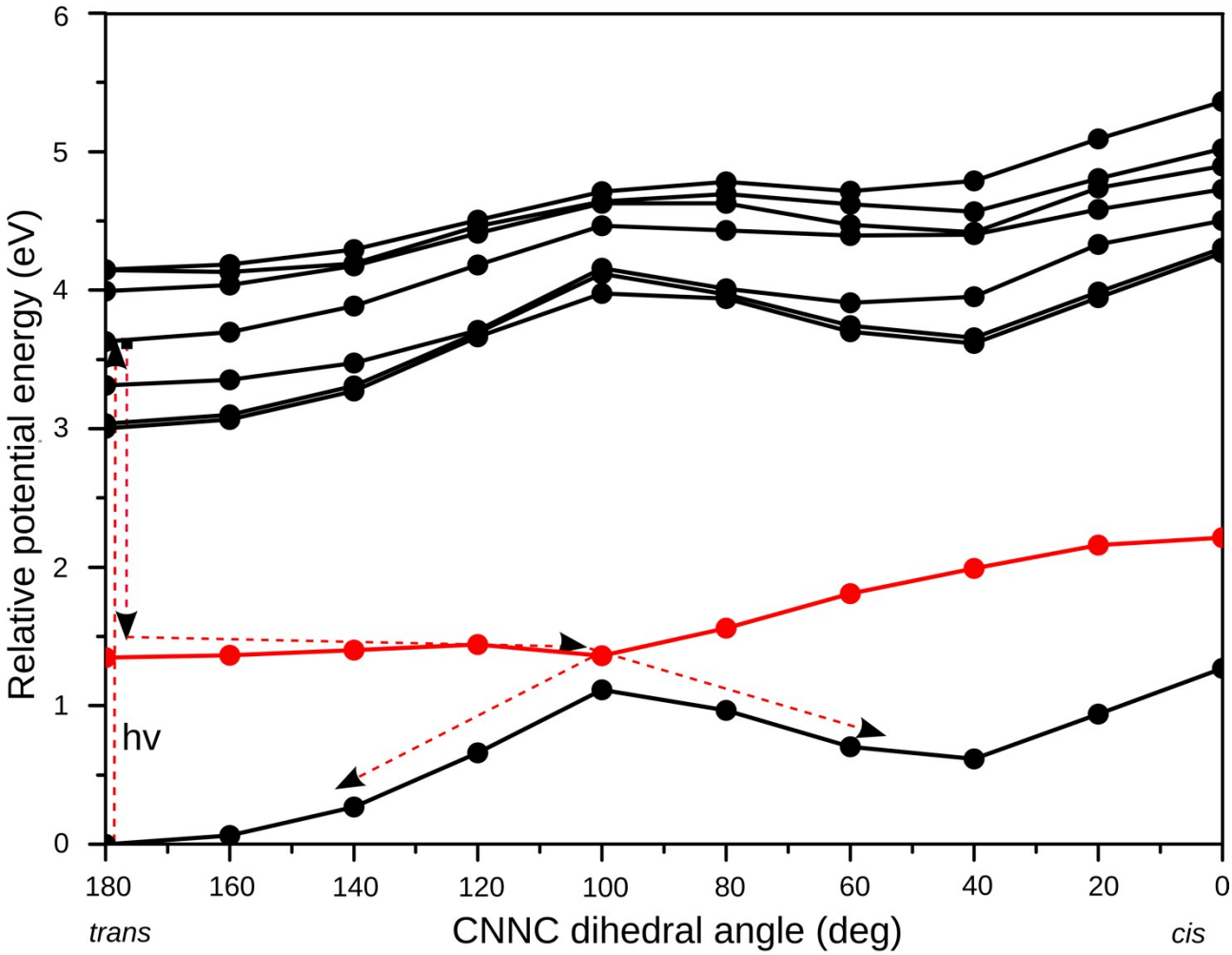

Figure S7: Relaxed scans of the potential energy surfaces along the isomerization pathway of the 2',4',6'-tri-CN substituted AB branch of (2',4',6'-tri-CN-4''-SH)-MTA after unconstrained relaxation of S_5. Initially, the excited S_5 $\pi\pi^*$ state decays into the S_1 $n\pi^*$ state localized at the 2',4',6'-tri-CN substituted AB branch, which undergoes barrierless isomerization along the CNNC dihedral angle rotation.