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Redesigning donor–acceptor Stenhouse adduct photoswitches through a joint experimental and computational study†

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Reporter: Kai An

Date: 2021-01-28

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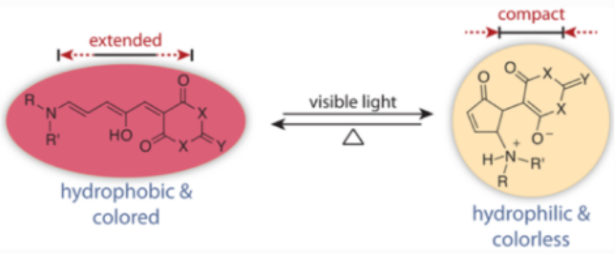
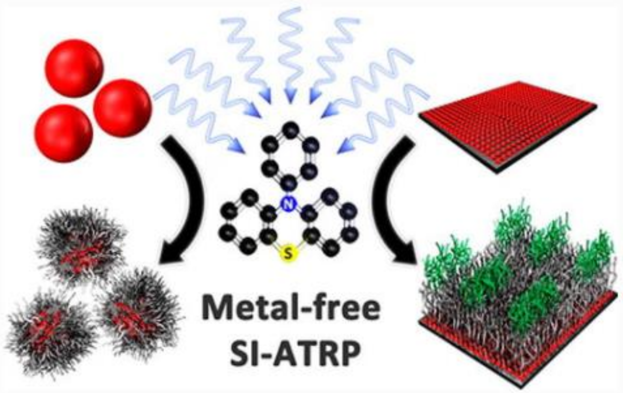
Light-Responsive Materials

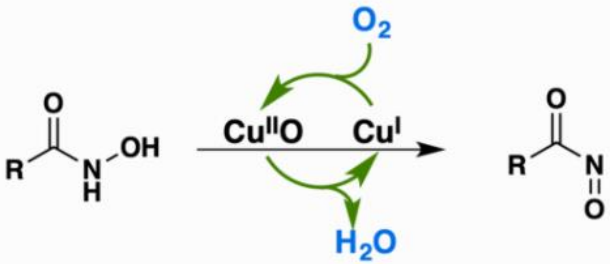


Donor–Acceptor Stenhouse Adducts DASAs

Synthesis of Polymers and Biomaterials

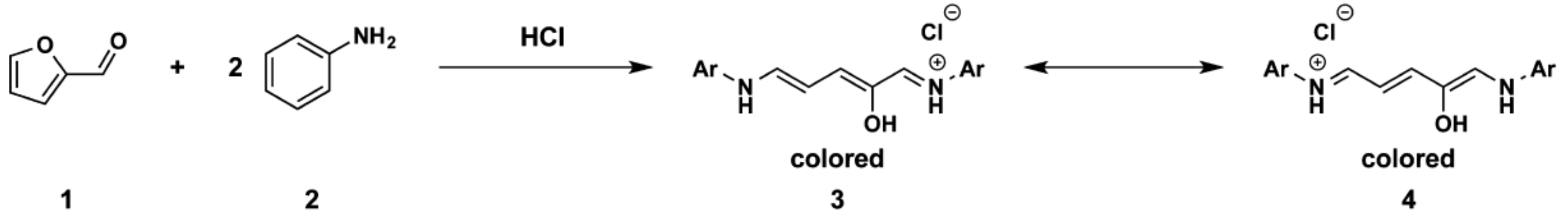


Copper Metal Catalysis

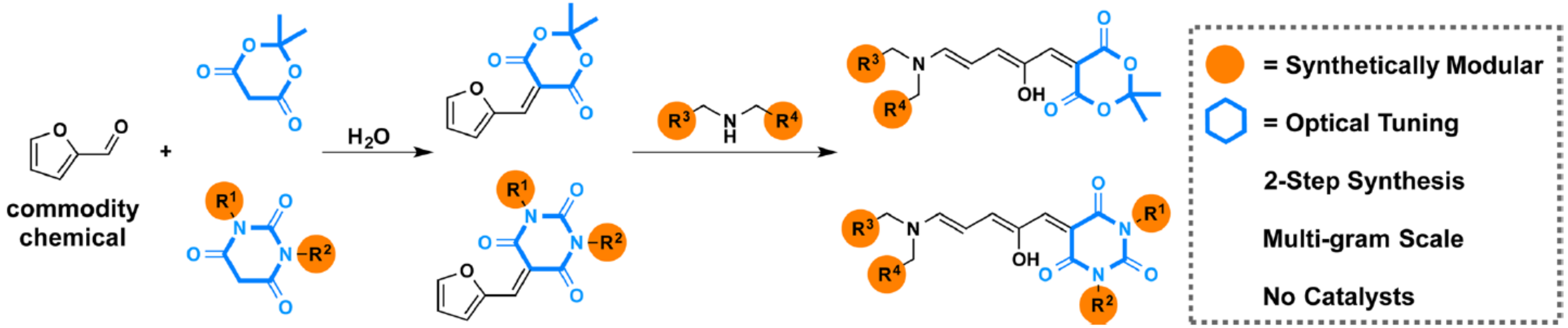


Donor–Acceptor Stenhouse Adducts (DASAs)

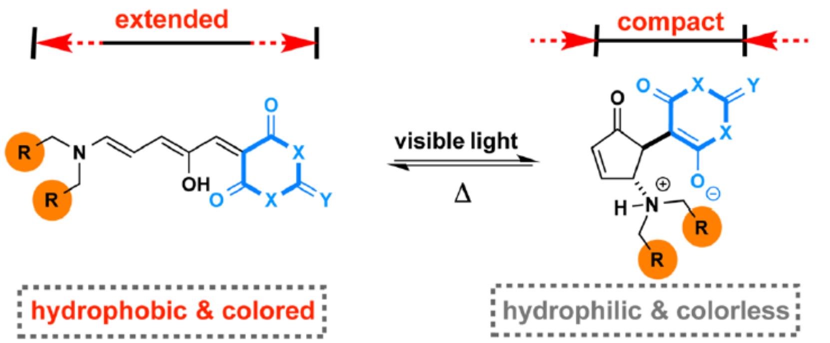
Stenhouse - 1870

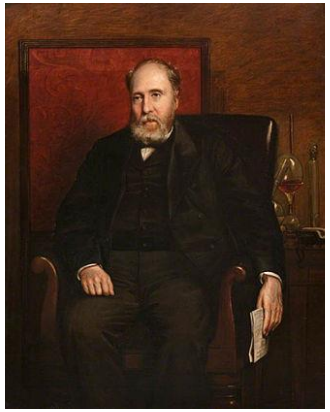


Design of the donor-acceptor Stenhouse adducts



Stenhouse-based organic photochromic material





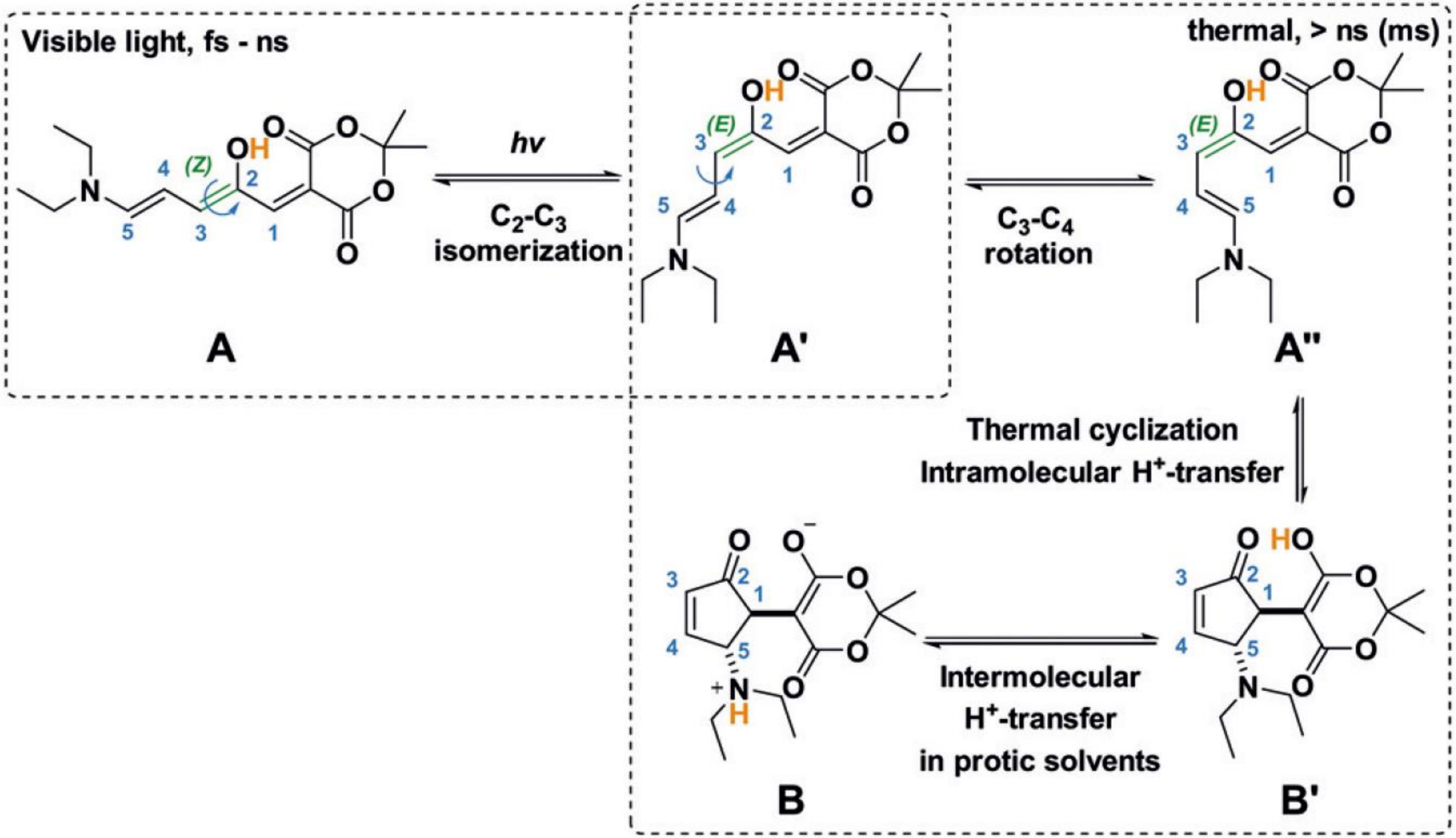
John Stenhous

（1809-1880）

J. Am. Chem. Soc. **2014**, 136, 8169−8172

J. Org. Chem. **2014,** 79, 11316–11329

Proposed Photoswitching Mechanism of DASAs



Ben Feringa

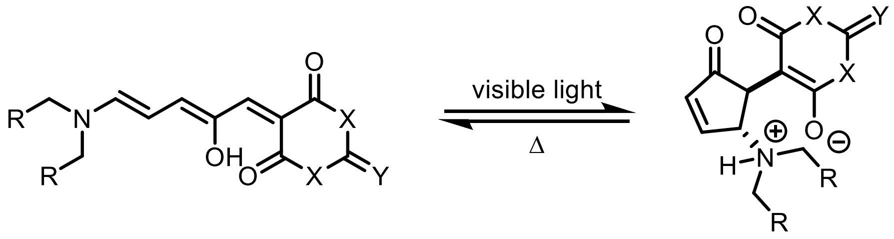
J. Am. Chem. Soc. **2016**, 138, 6344−6347

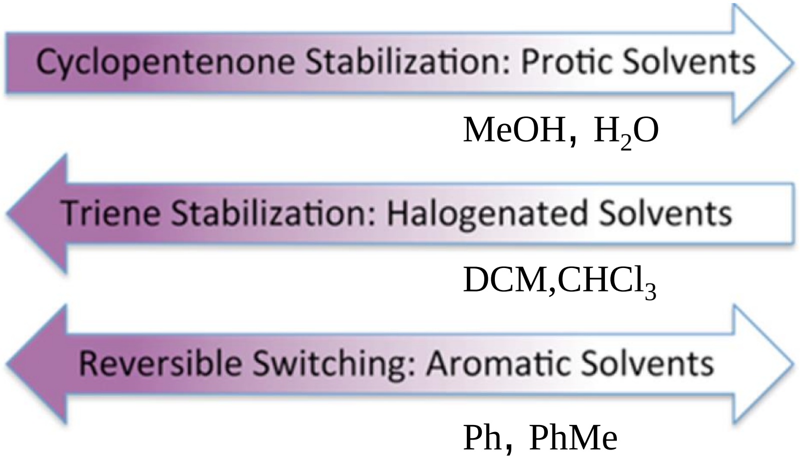
Angew. Chem. Int. Ed. **2018,** 57, 8063 –8068

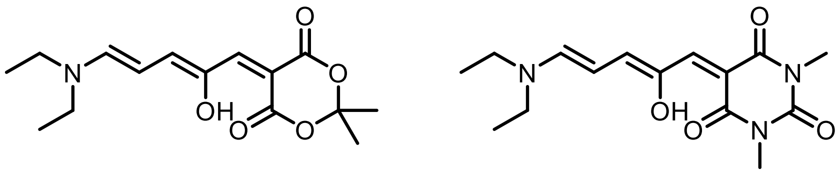
J. Am. Chem. Soc. **2019**, 141, 7376−7384

Donor–Acceptor Stenhouse Adducts (DASAs)

➢ first generation







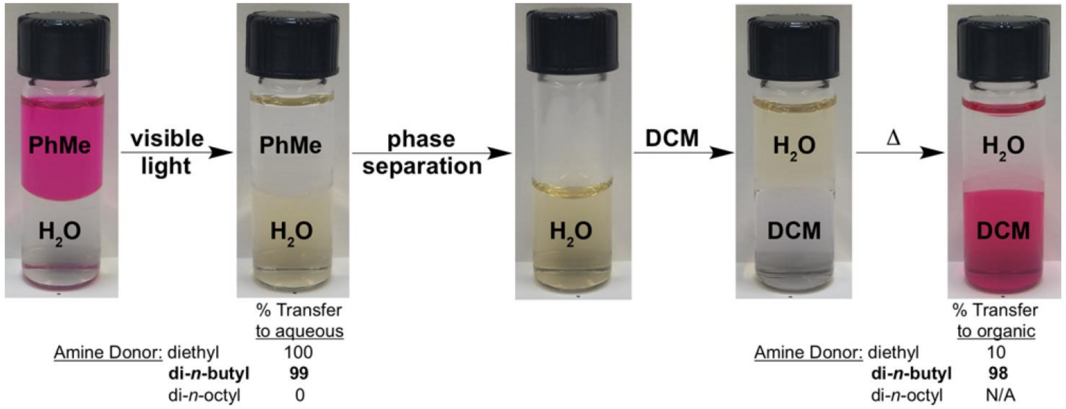
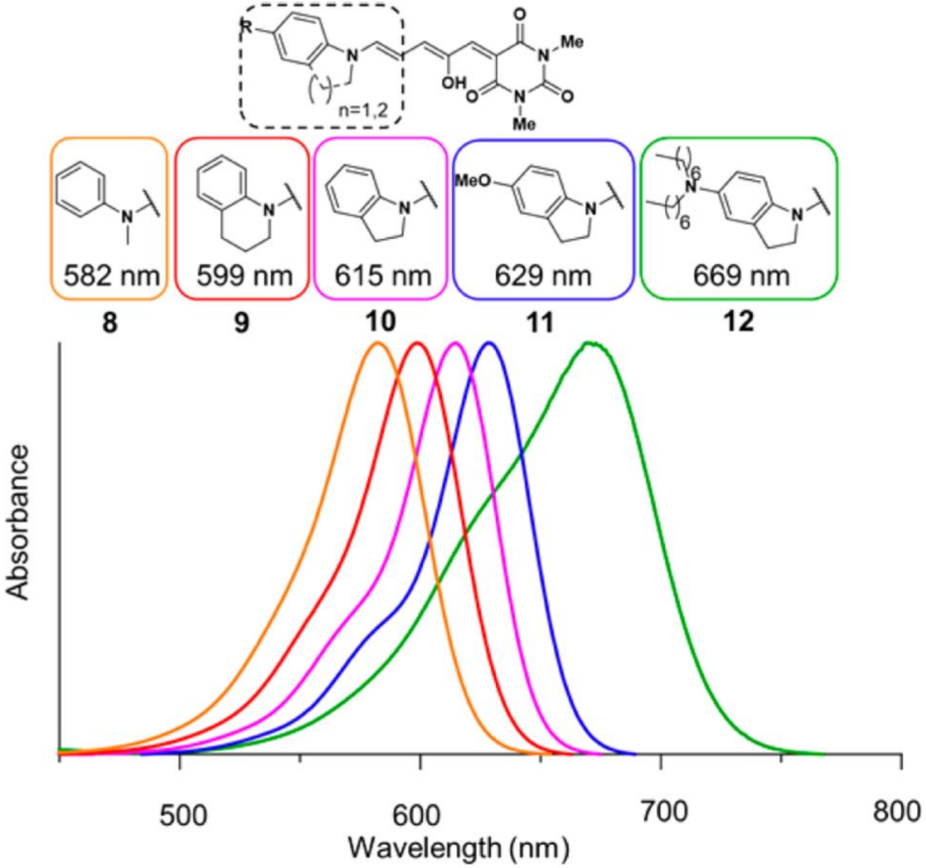


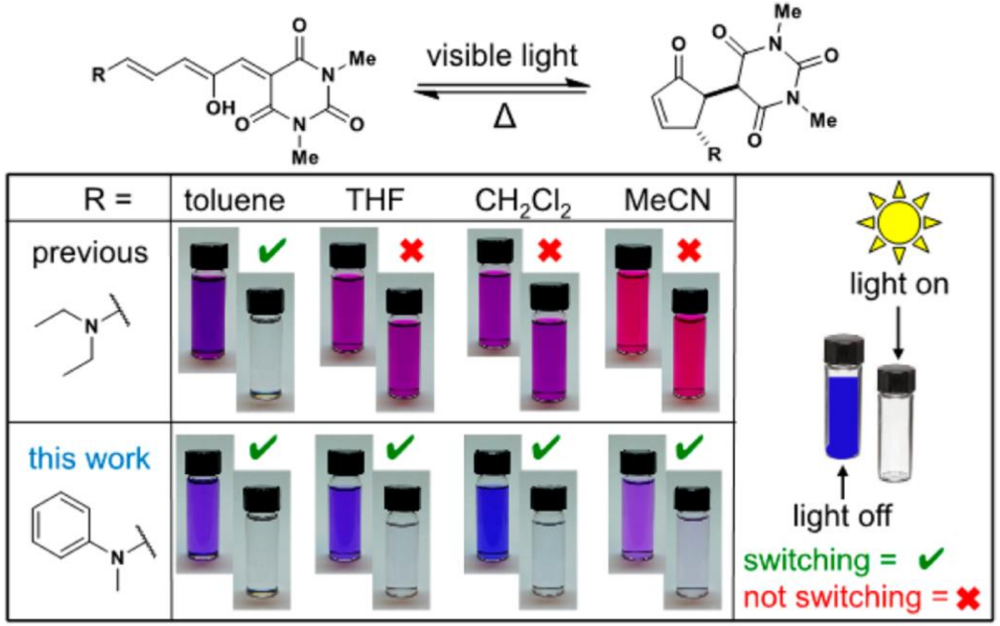
Figure . Schematic representation of DASA dynamic phase transfer and results

J. Org. Chem. **2014,** 79, 11316–11329

Donor–Acceptor Stenhouse Adducts (DASAs)

- **second generation**

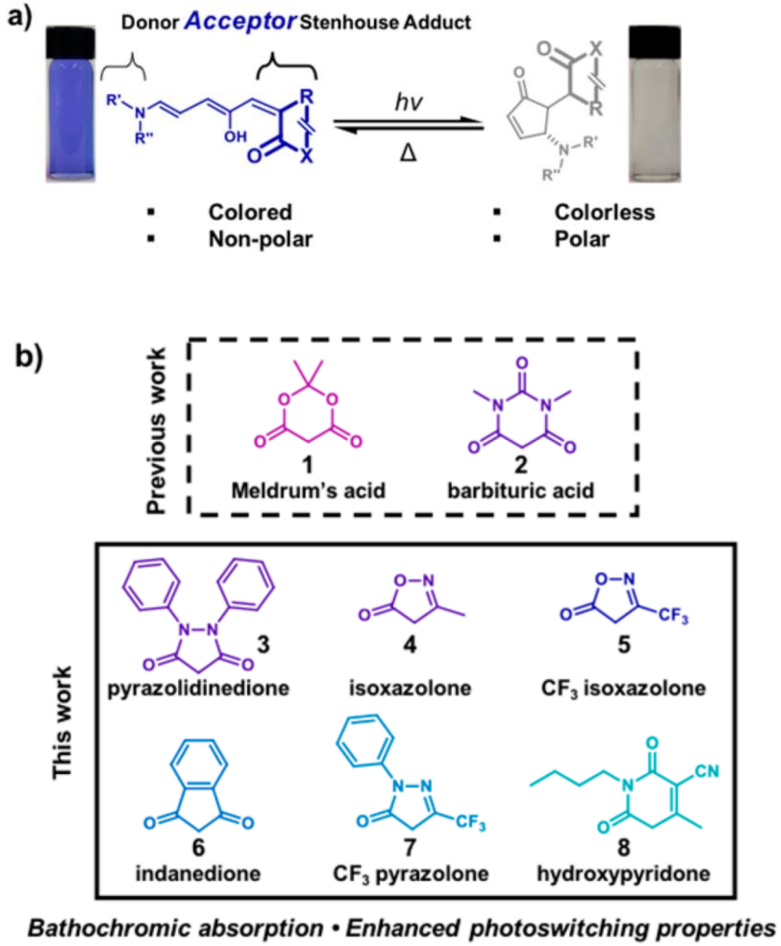


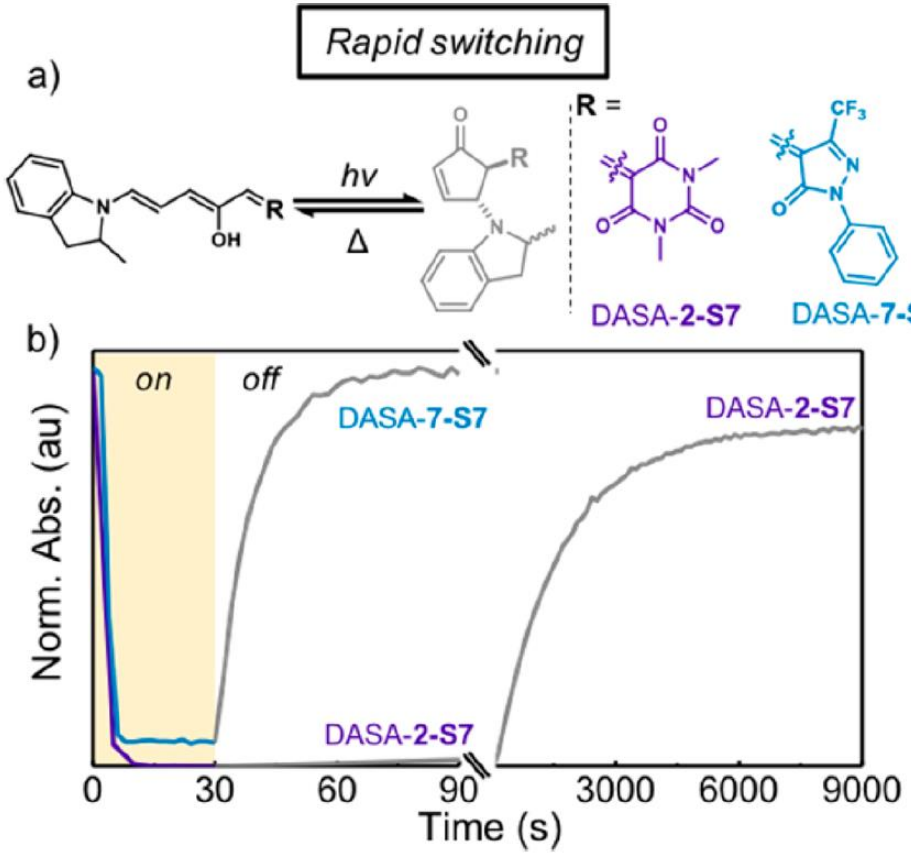


J. Am. Chem. Soc., **2016,** 138, 13960–13966

Donor–Acceptor Stenhouse Adducts (DASAs)

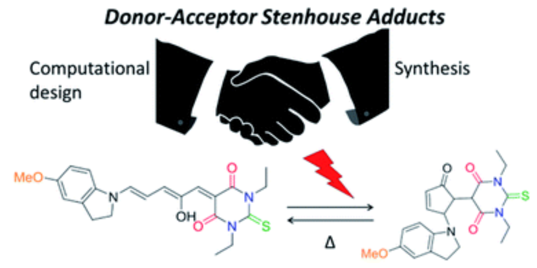
- **third generation**

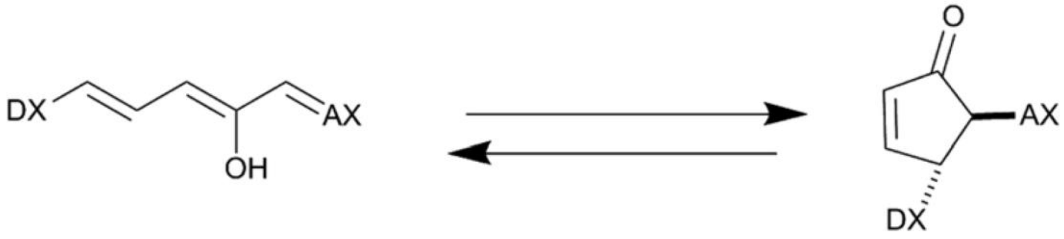




J. Am. Chem. Soc. **2018**, 140, 10425−10429

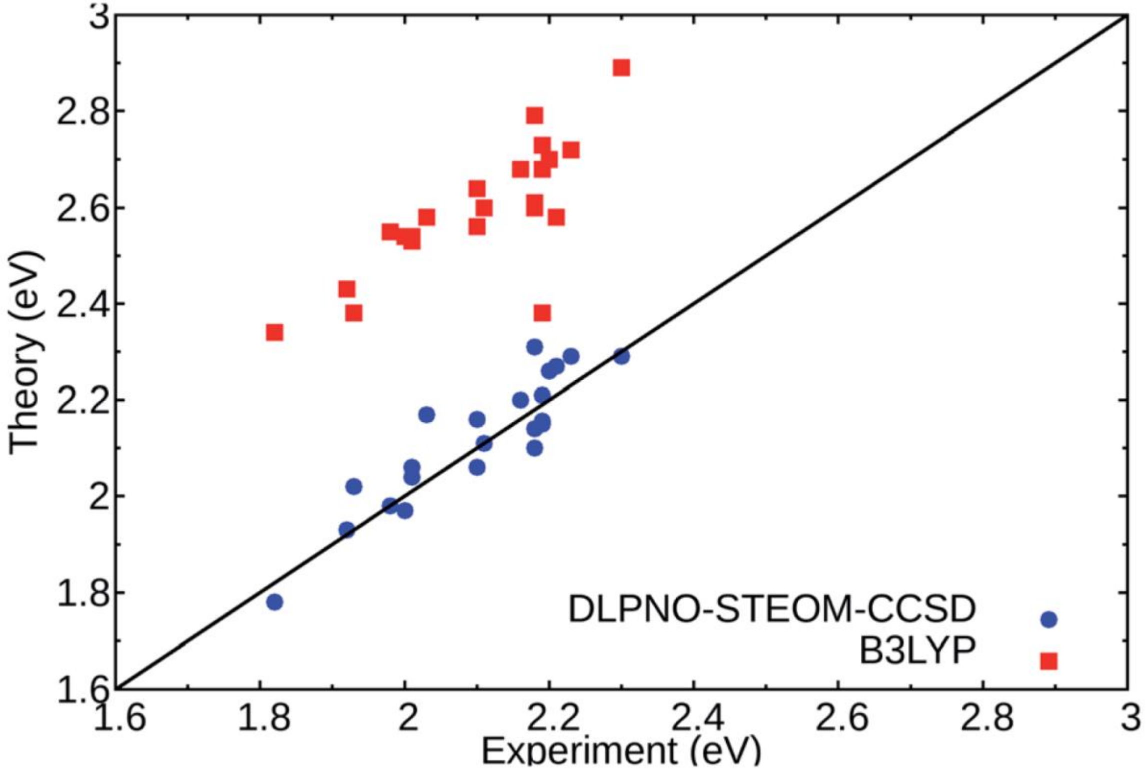
Benchmarking the Recommended Protocol

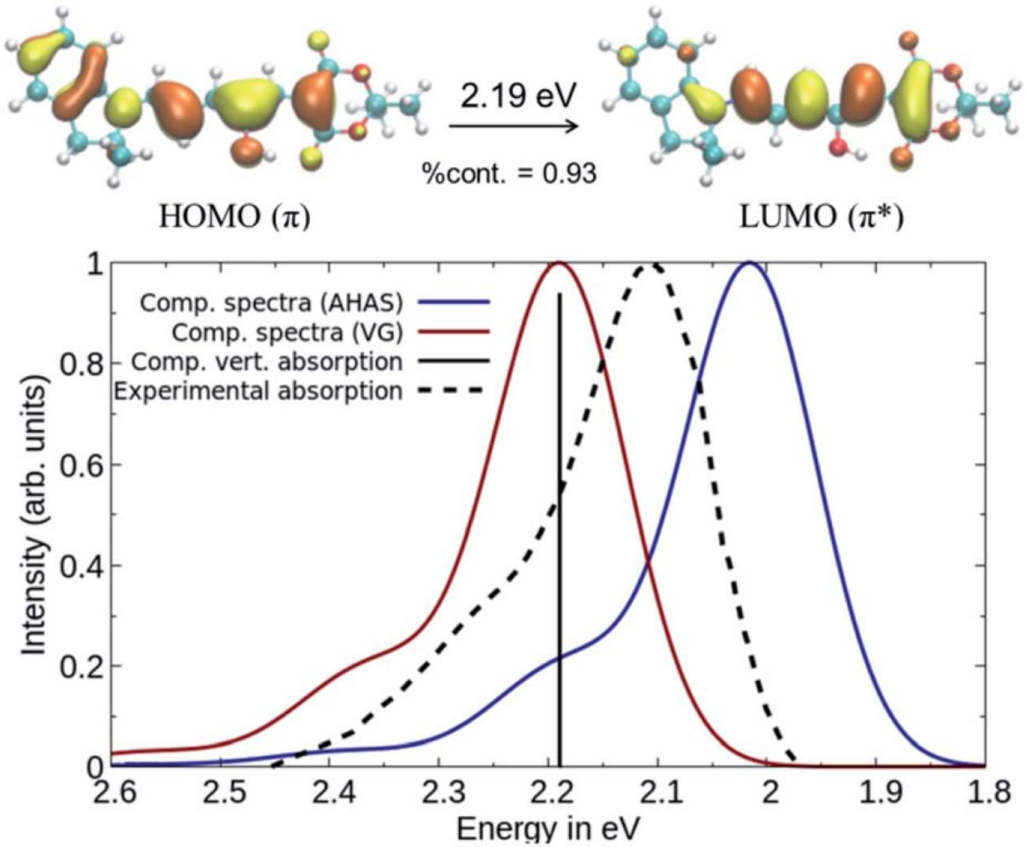




Open form (colored)

Closed form (colorless)





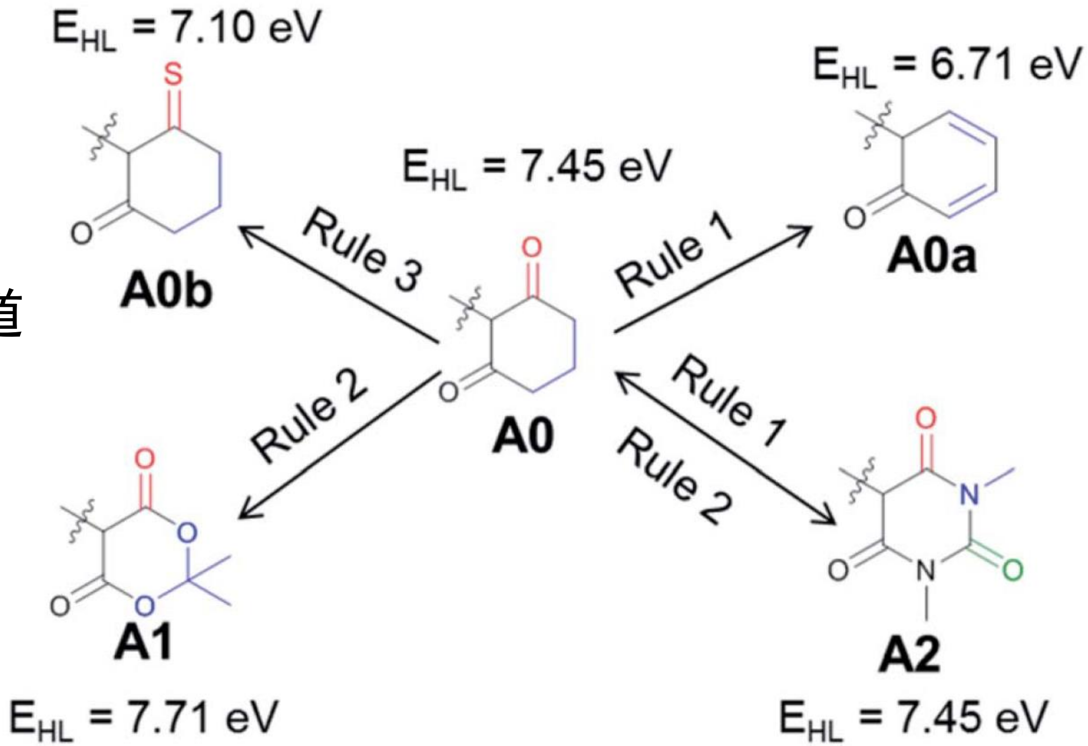
Computational Design of New DASAs

染料光谱红移经验：

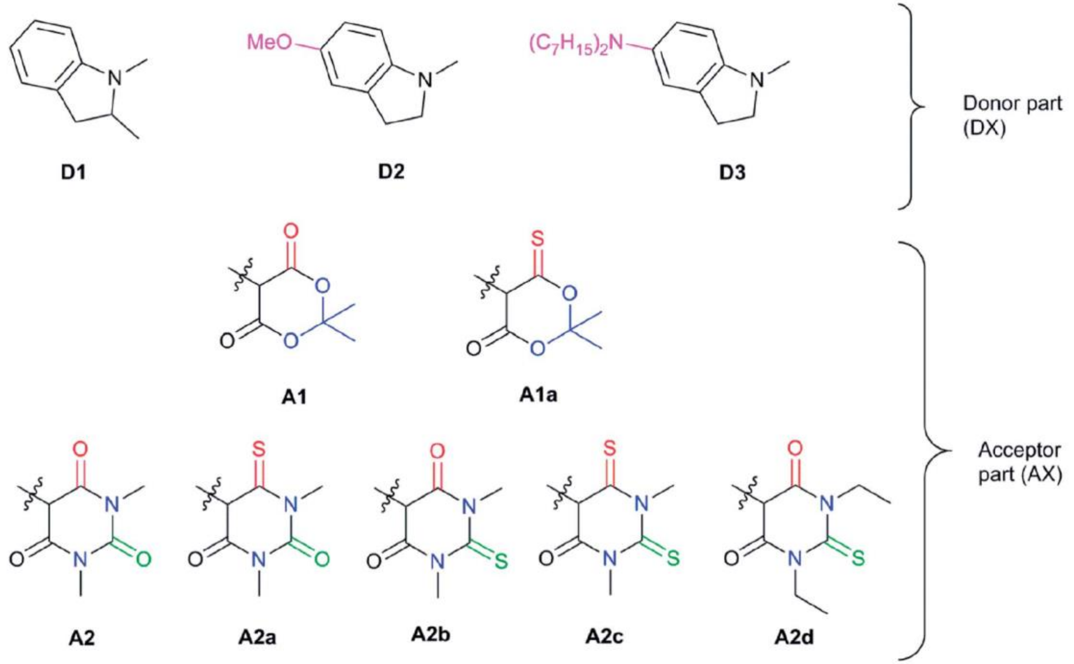
Rule 1.延长共轭体系

Rule 2. 供/吸电子基团不稳定/稳定分子轨道

Rule 3. 同族元素取代氧



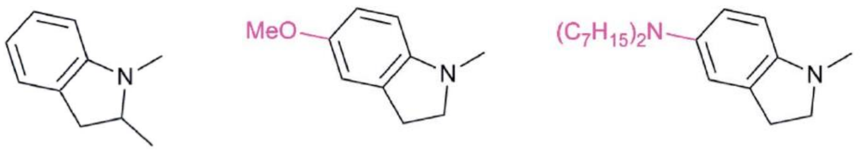
Computational Design of New DASAs



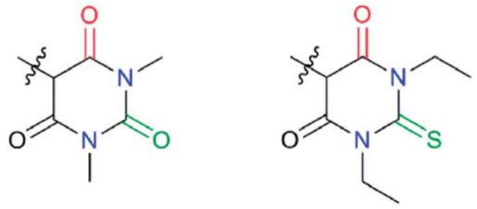
1A → 2A transition	Comp. VEE (eV)	Comp. E_{max} (eV)	Exp. E_{max} (eV) in CH_2Cl_2
D1–A1	2.19	2.18	2.1
D1–A1a	1.88	1.89	—
D1–A2	2.00	1.97	2.02
D1–A2a	1.75	1.75	—
D1–A2b	1.89	1.89	—
D1–A2c	1.64	1.64	—
D1–A2d	1.84	1.85	1.92
D2–A2d	1.80	1.80	1.88
D3–A2d[a]	1.72	1.72	1.77

[a] For the computational results $N(Me)_2$ was considered instead of $N(C_7H_{15})_2$ in the donor part.

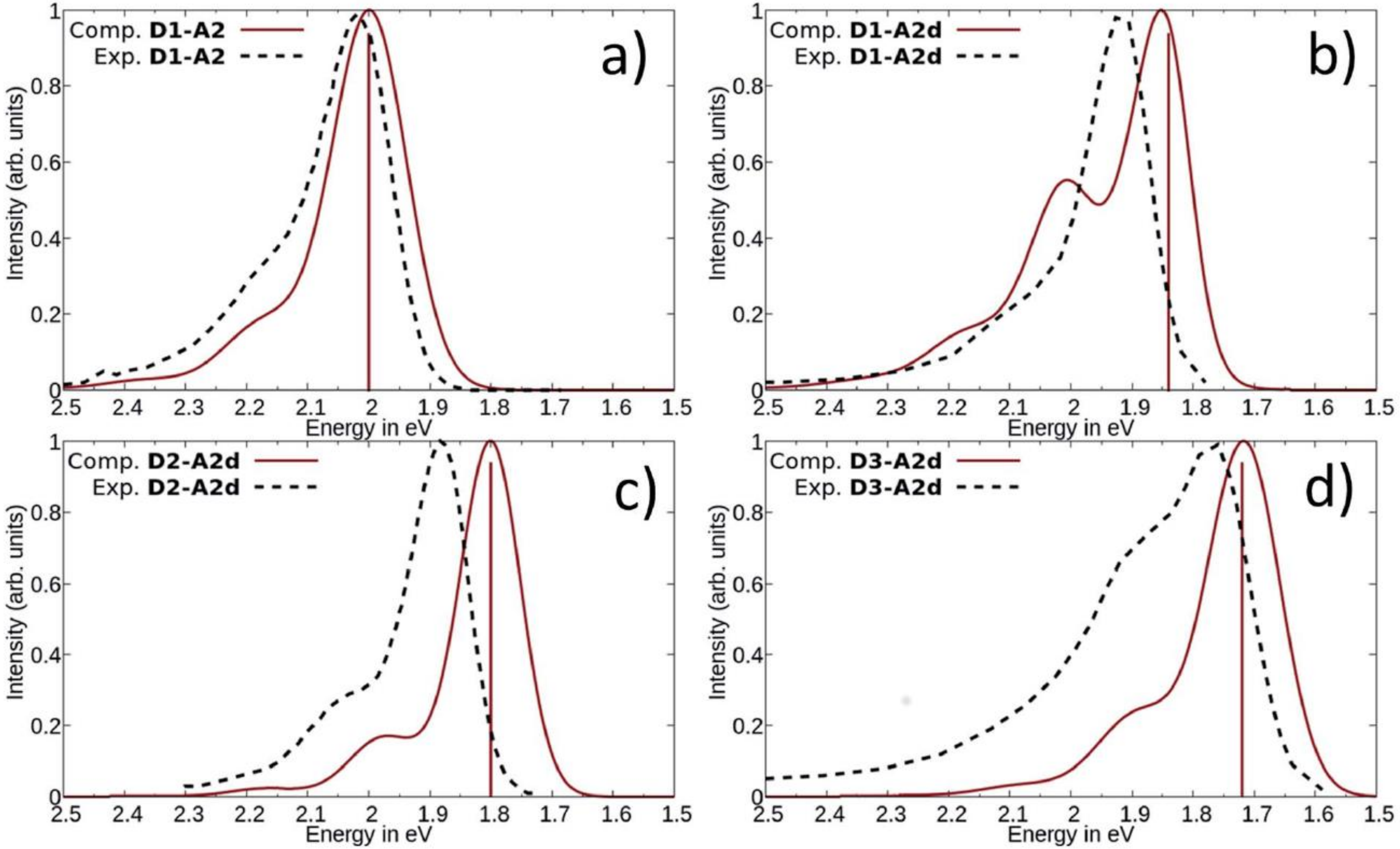
Comparison between computed and experimental absorption spectra of DASAs



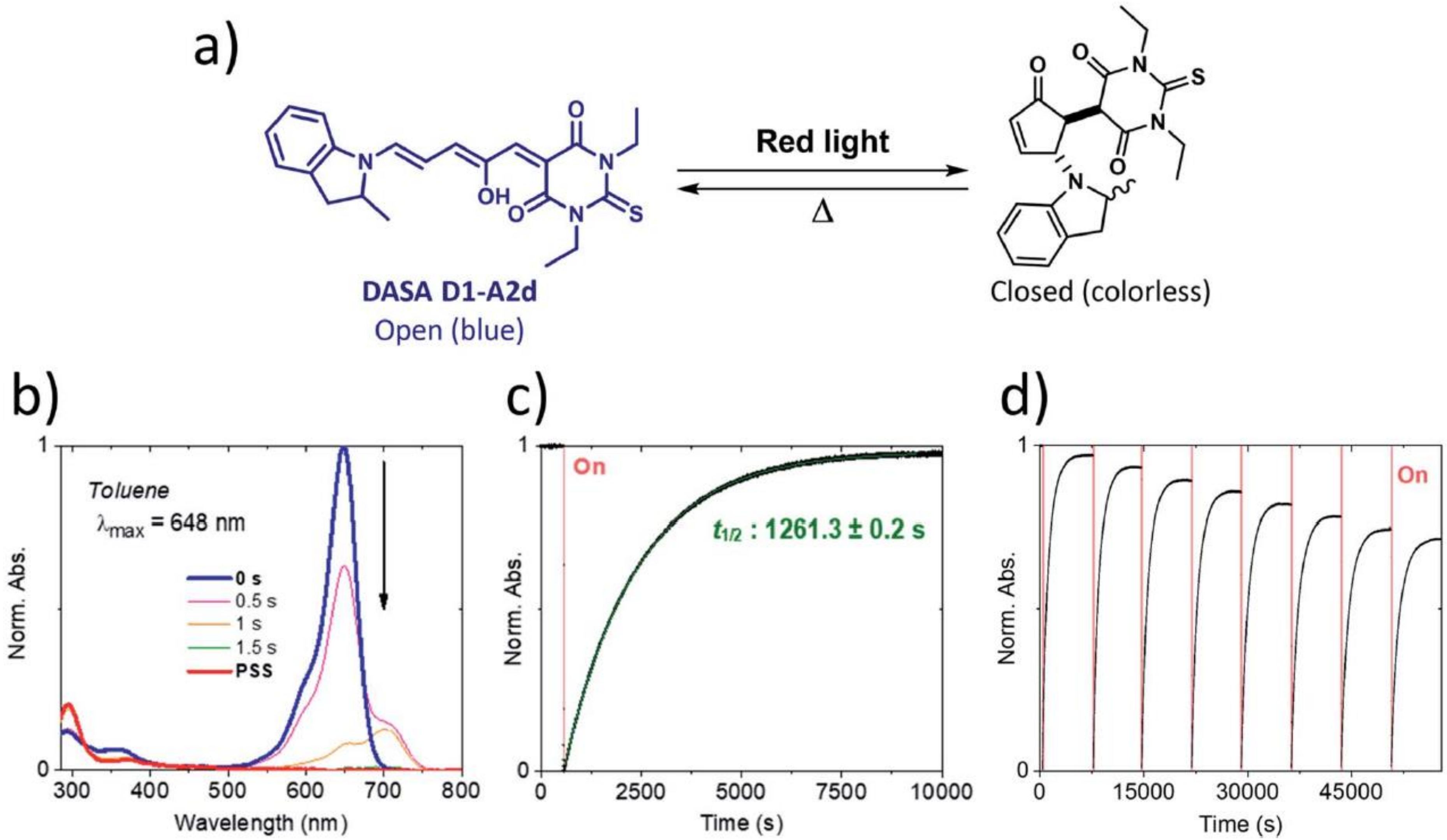
D1 D2 D3



A2 A2d



Photochromism of DASA D1–A2d in Toluene



Photochromism of DASA D1–A2d and D3-A2d in Toluene