BiOrgaMCT
Bioactive Organic and inorganic advanced Materials and Clean Technologies

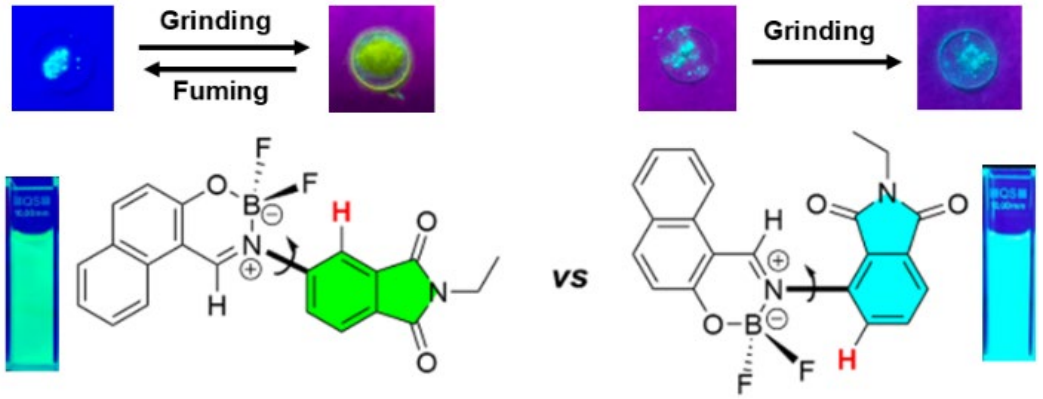
Funded by the European Union
NextGenerationEU

MINISTRY OF EDUCATION AND SCIENCE

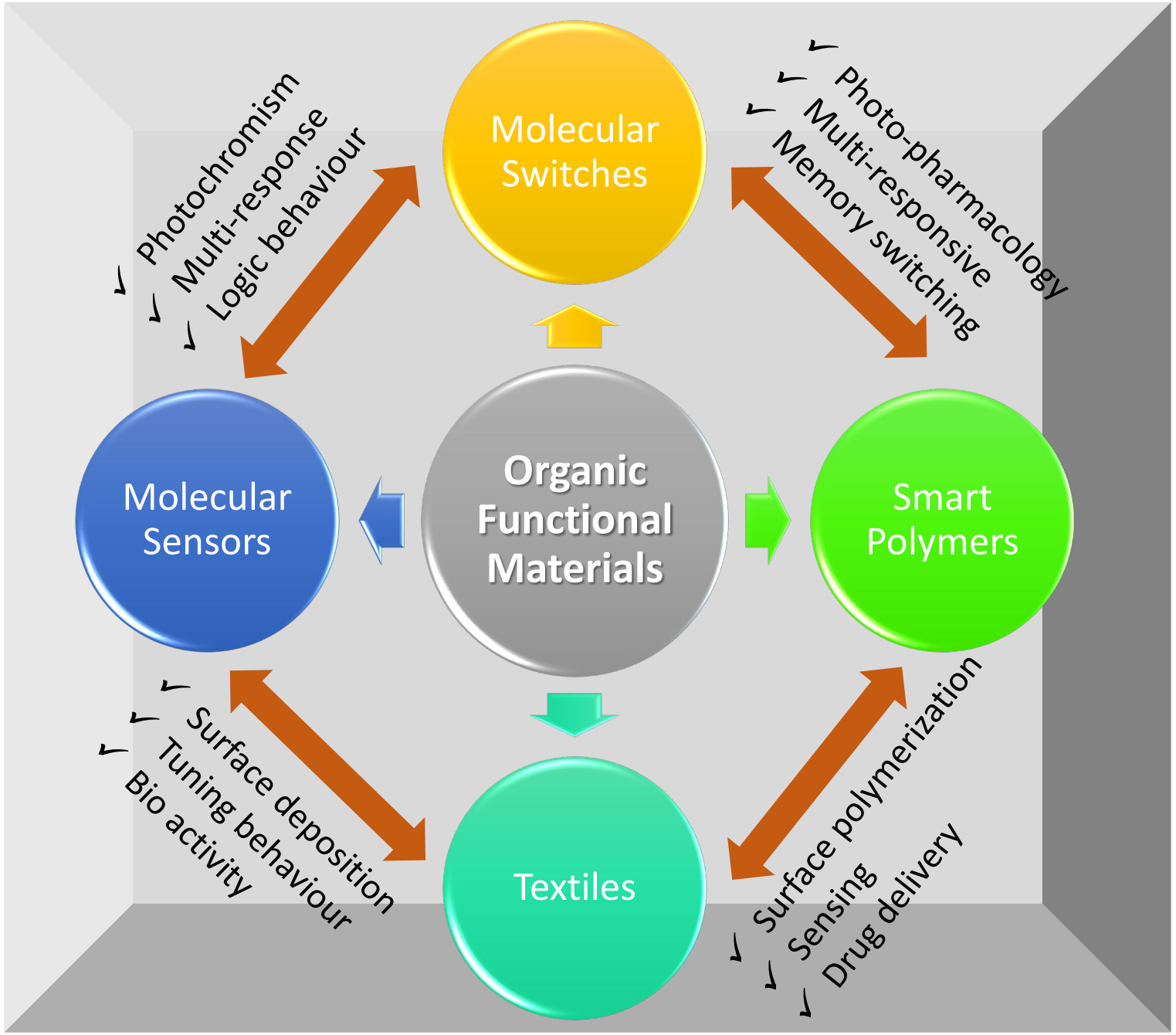
Organic Functional Materials

Part of the project №BG-RRP-2.004-0002, "BiOrgaMCT"

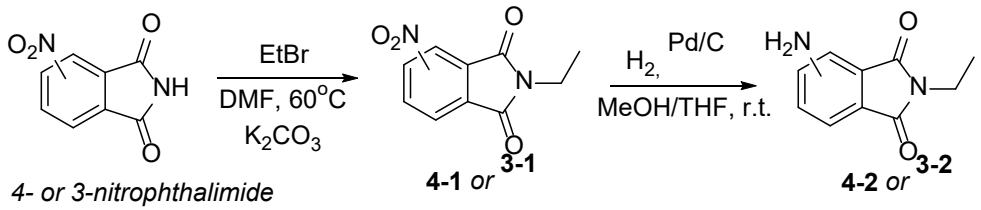
Excited-state dynamics in 4- and 3-substituted Phthalimide Boron Difluoride Complexes

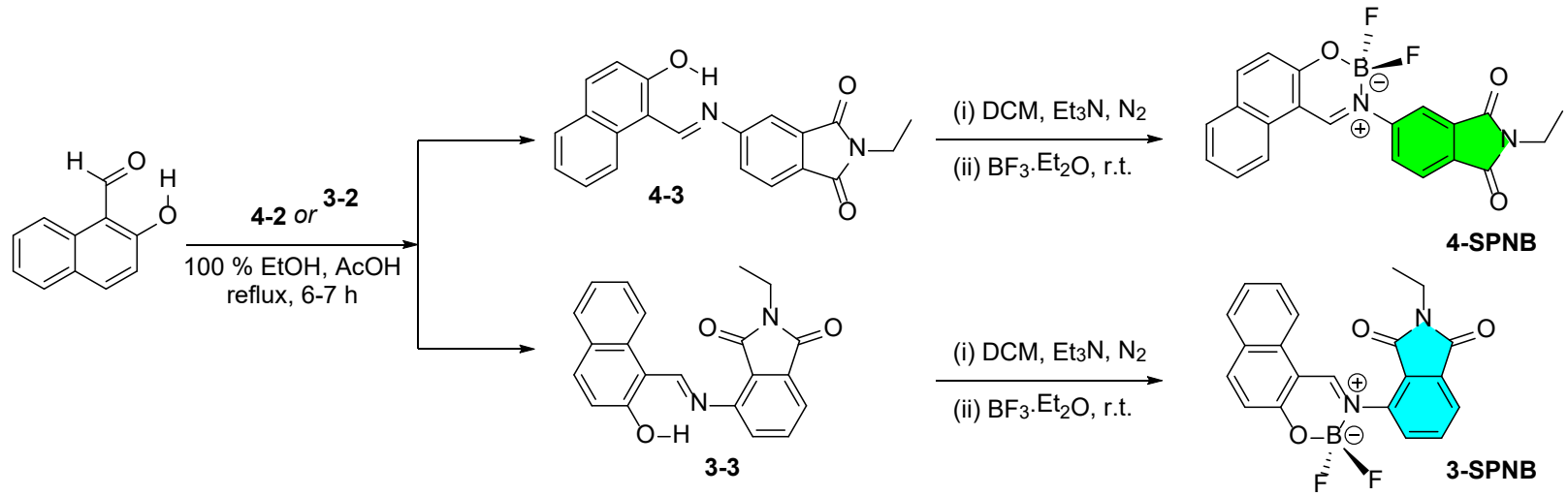


State-of-the-art

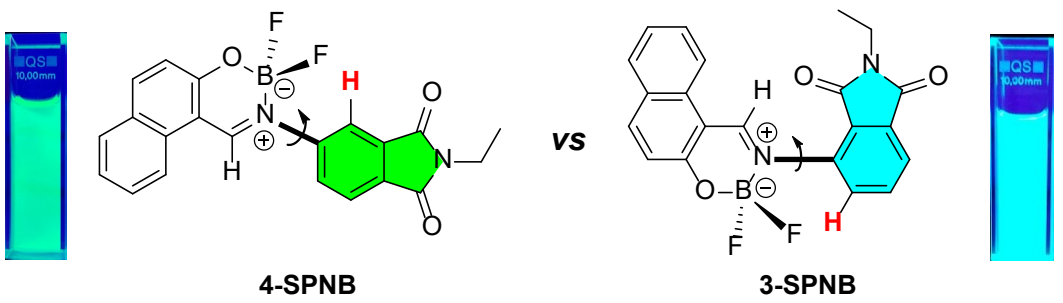


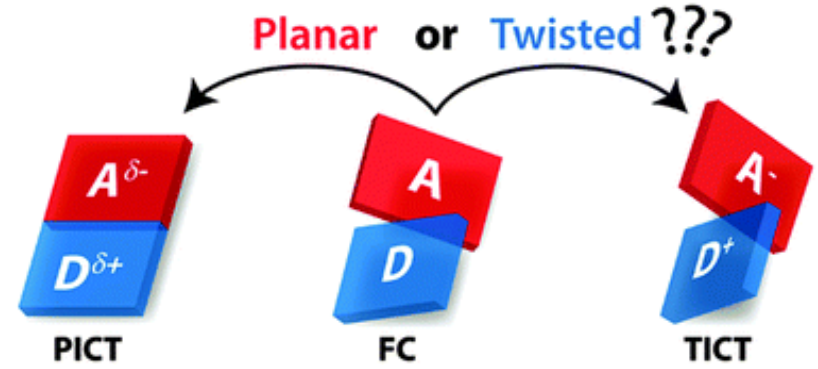
The synthesis of Phthalimide Boron Difluoride Complexes

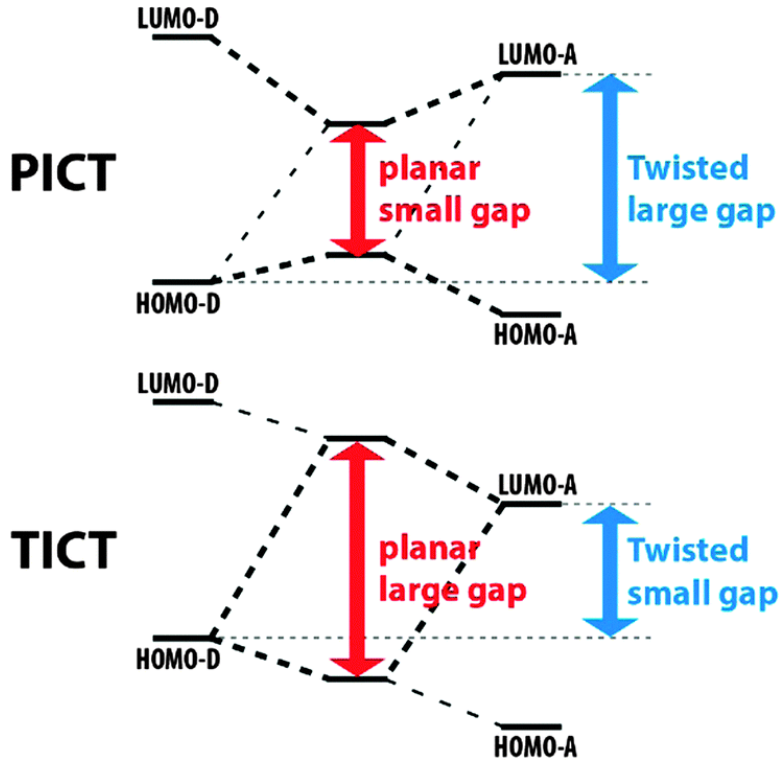




Fluorescent Rotary Switches

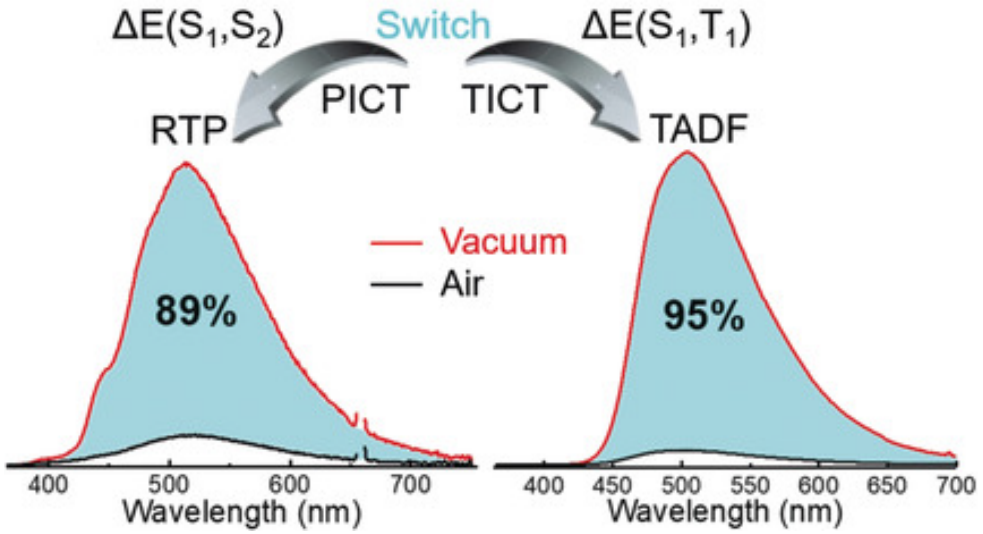




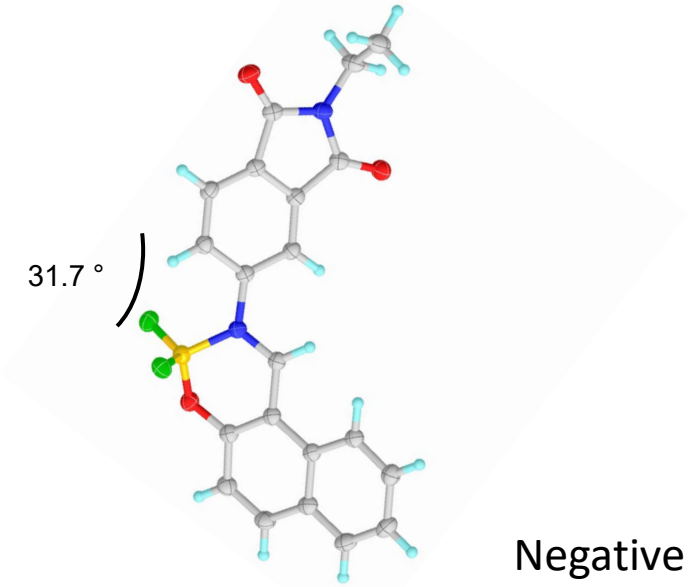


Ref: Phys. Chem. Chem. Phys., 2015,17, 9248-9257

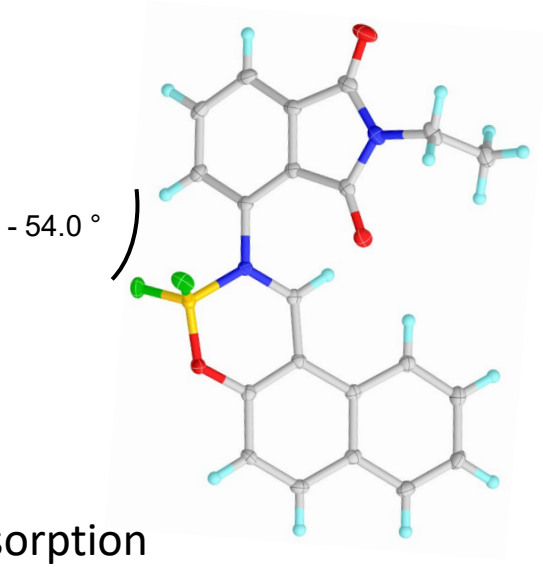
State-of-the-art & Theory



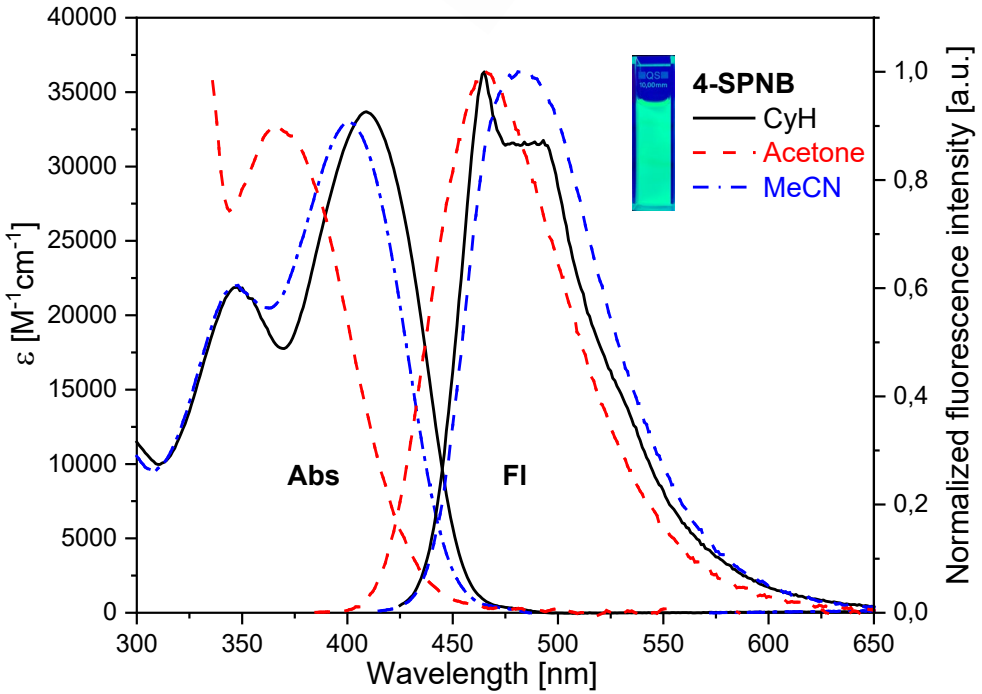
Ref: Angew. Chem. Int. Ed. 2018, *57*, 16407

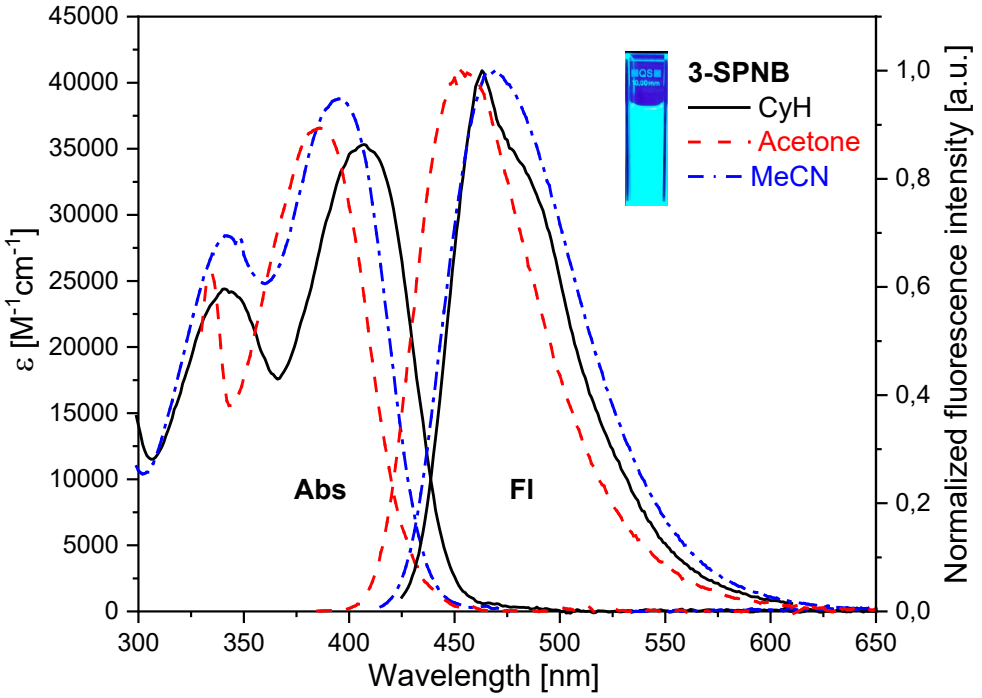


X-Ray structures

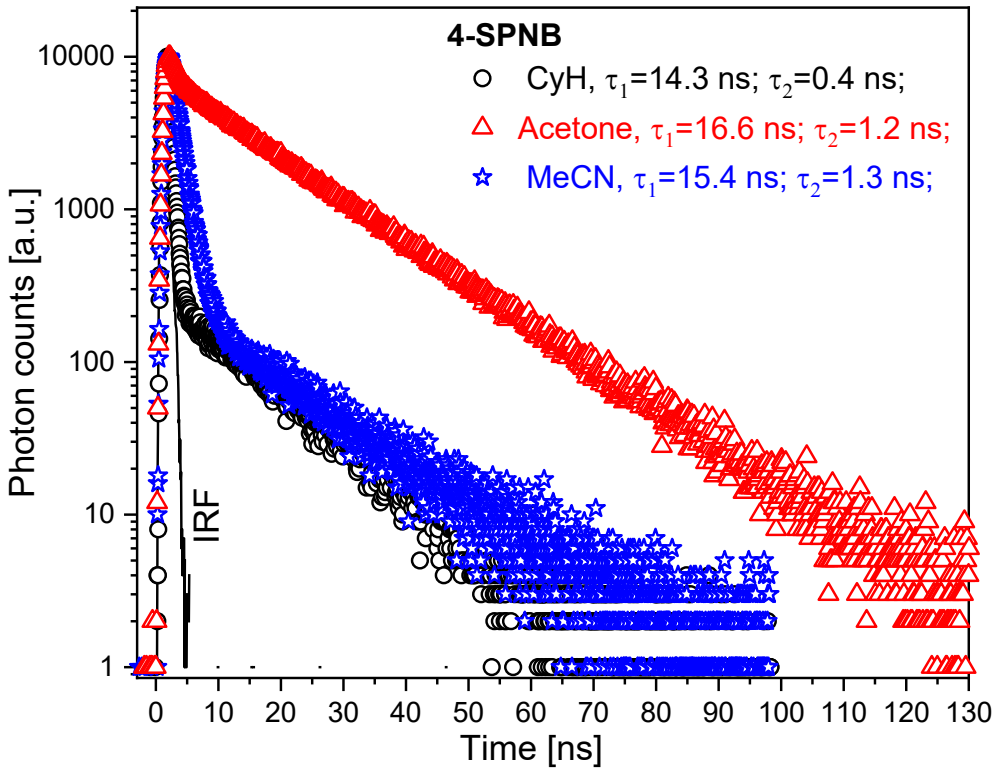


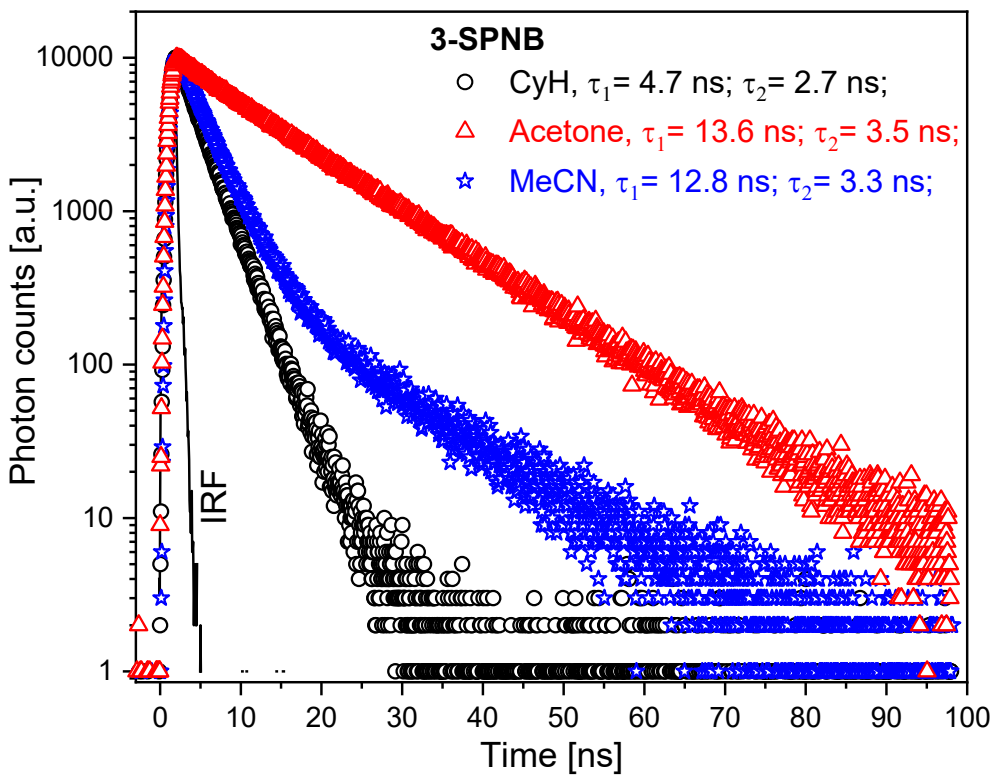
Negative solvatochromism in absorption





Steady-state absorption and emission



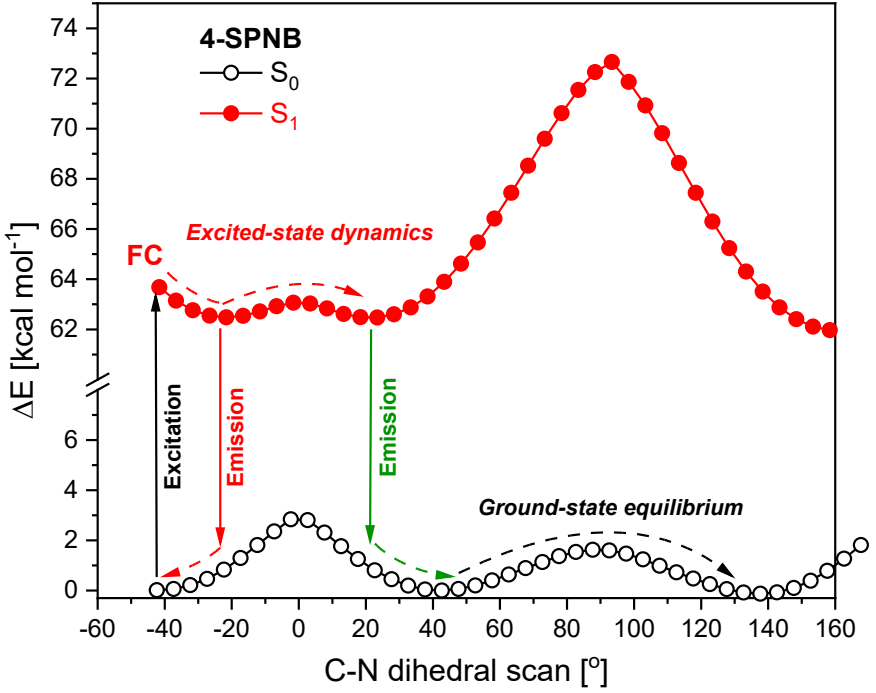


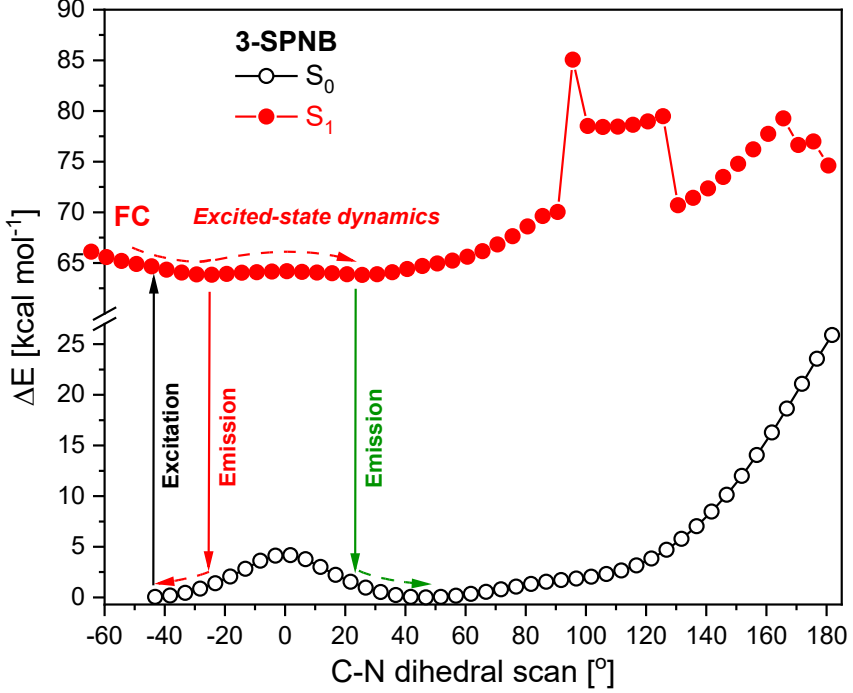
Time-correlated Single Photon Counting (TCSPC) measurements.

- ✓ *We have used picosecond NanoLed laser at 390 nm as excitation source.*
- ✓ *The fittings were performed by double exponential decay function.*

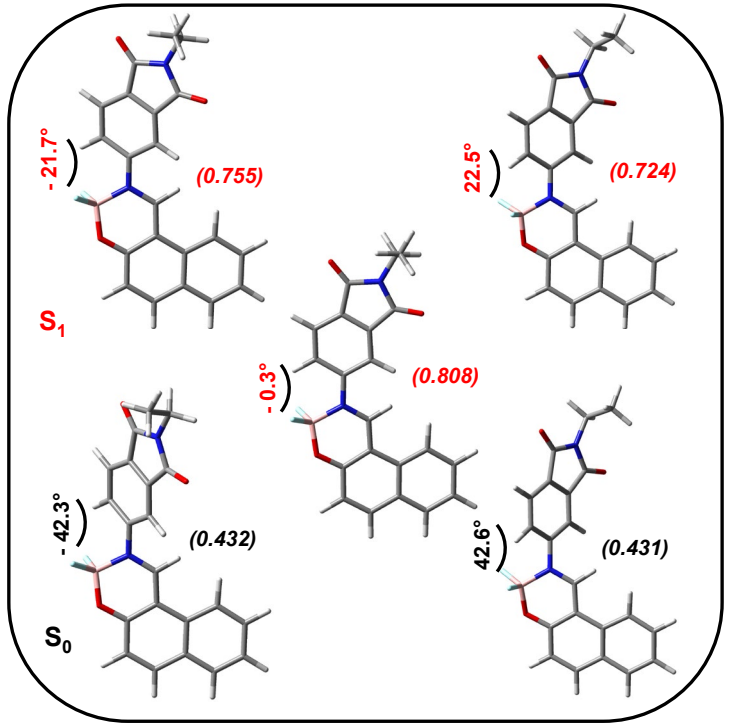
Photophysical data

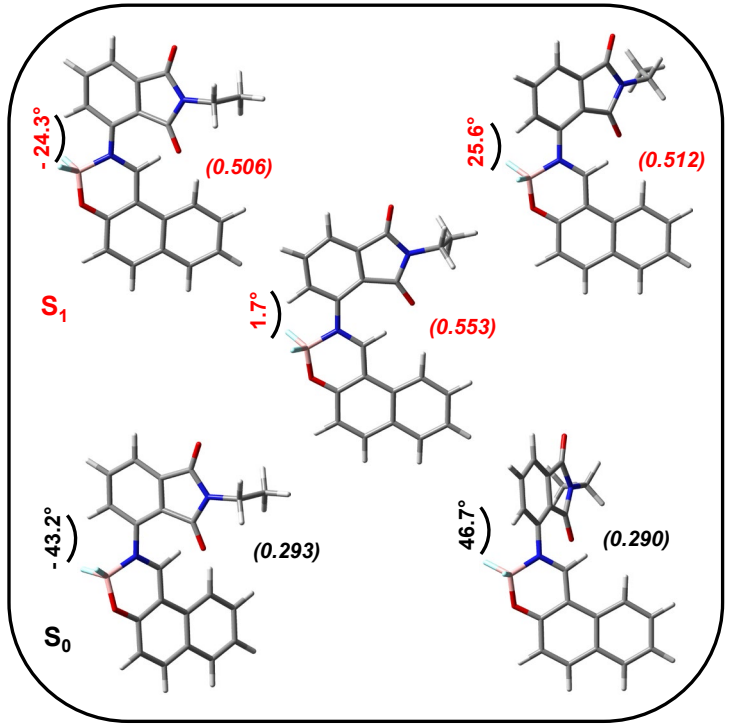
Solvents	4-SPNB					3-SPNB				
	λ_{abs} [nm]	λ_{em} [nm]	[a] SS [cm^{-1}]	τ [ns]	Φ_{fl} [%]	λ_{abs} [nm]	λ_{em} [nm]	[a] SS [cm^{-1}]	τ [ns]	Φ_{fl} [%]
CyH	410	464, 493	2840	14.3 0.4	4.8	406	463	3030	4.7 2.7	38.0
DCM	409	478	3530	19.5 1.1	17.2	405	469	3370	12.2 3.1	36.3
THF	404	474	3650	14.2 1.1	15.2	400	468	3630	11.9 3.2	38.5
Acetone	366	466	5860	16.6 1.2	21.2	386	455	3920	13.6 3.5	35.4
MeCN	399	482	4320	15.4 1.3	19.3	395	468	3950	12.8 3.3	34.1



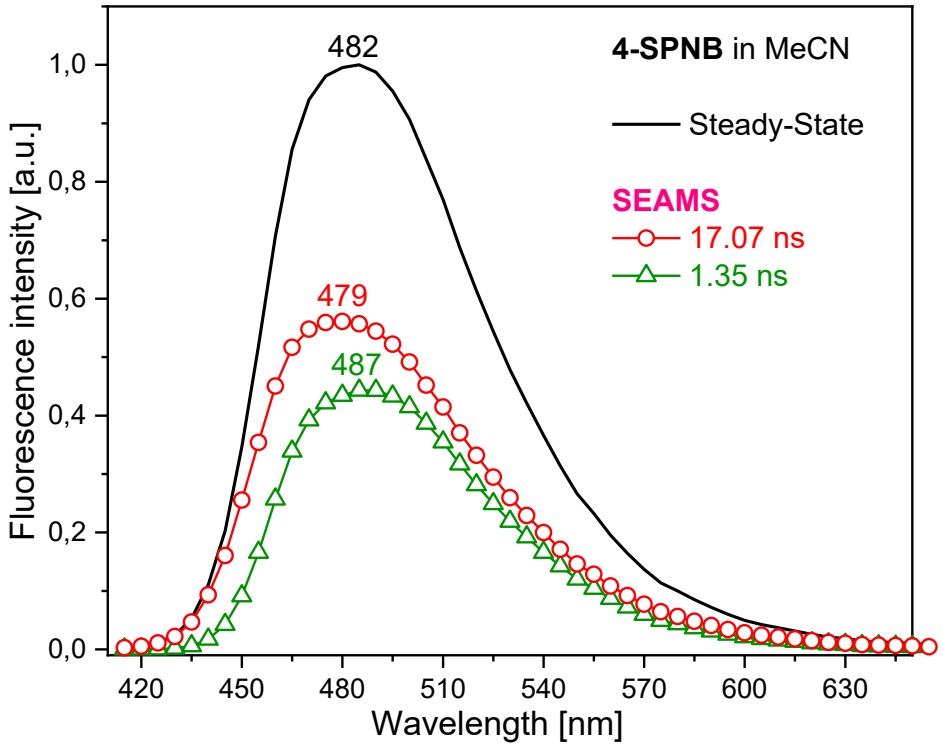


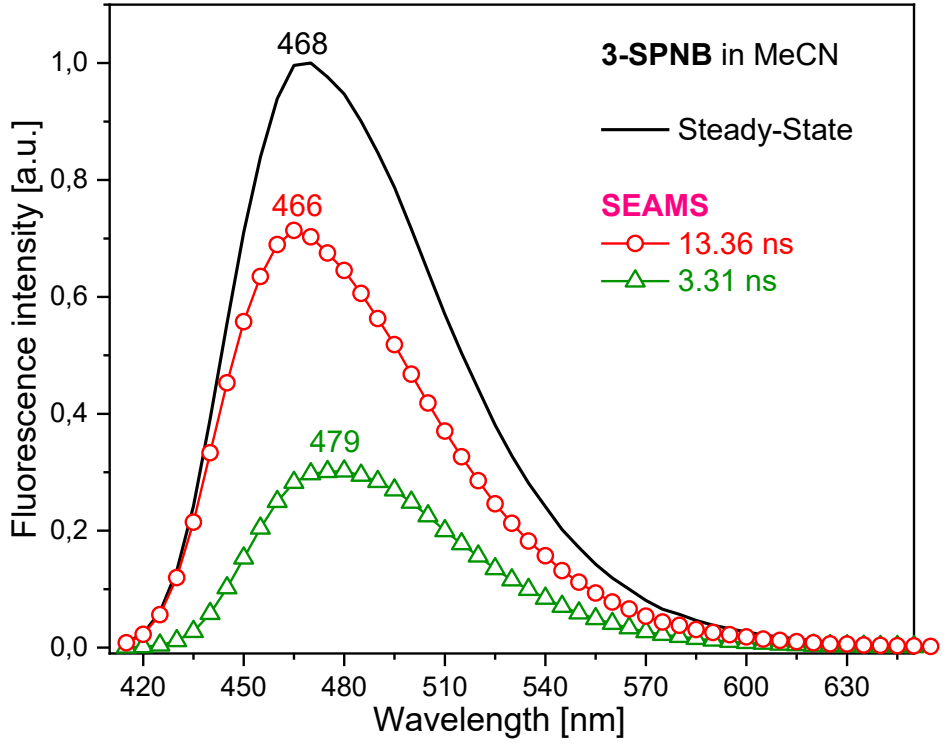
Ground and excited state DFT energy landscape of B-N-C-C dihedral angle





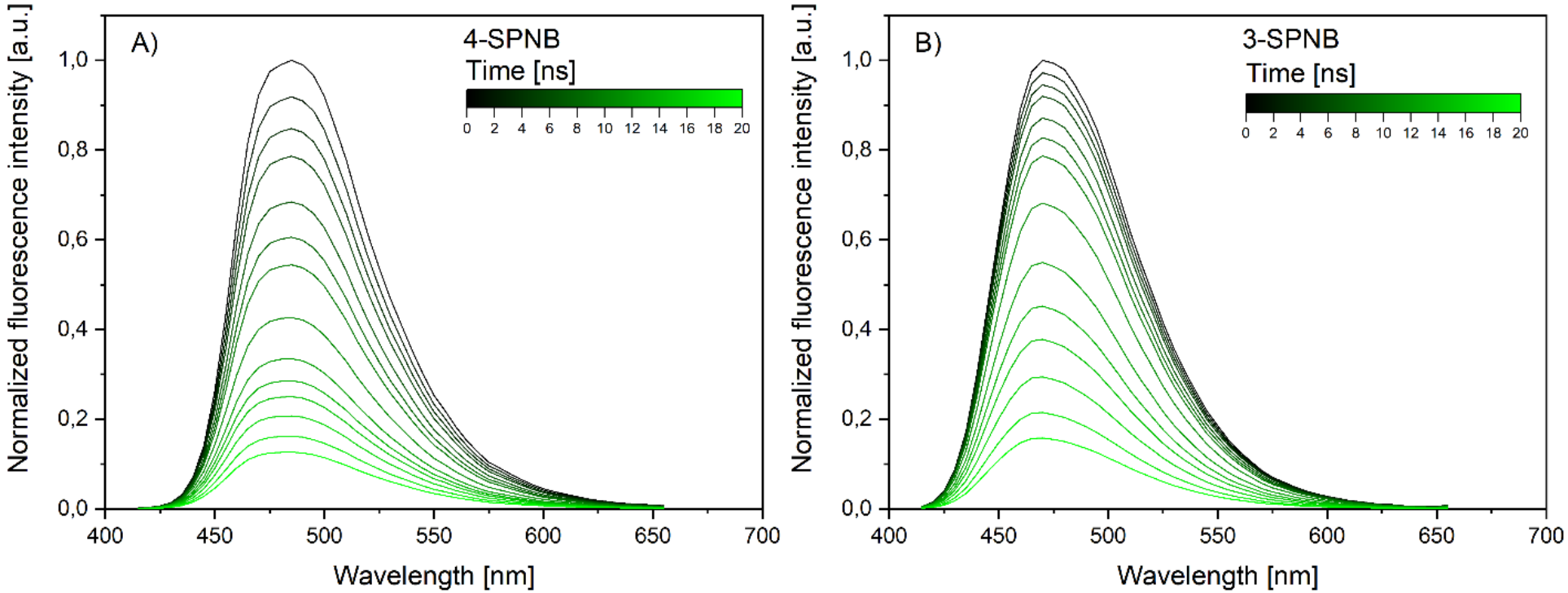
- ✓ *B3LYP/cc-pVDZ level of theory*
- ✓ *B-N-C-C dihedral angle scanning per 5° .*
- ✓ *The oscillator strengths are given in the brackets.*





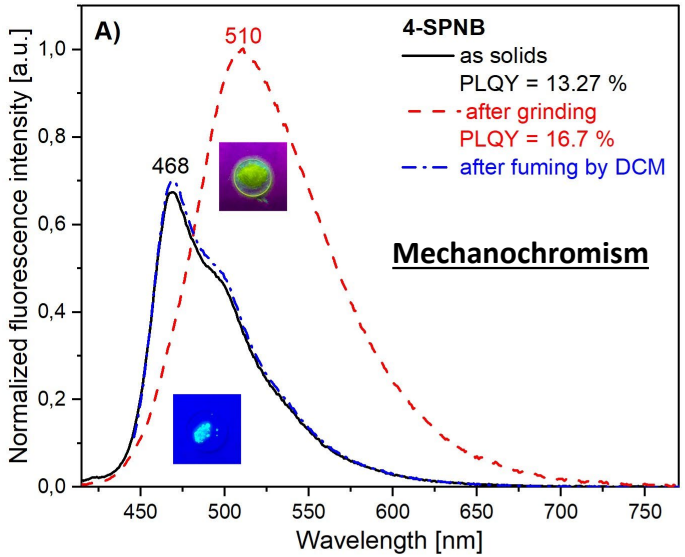
Comparison of the experimental steady-state and species-associated emission spectra (SAEMS) in MeCN.

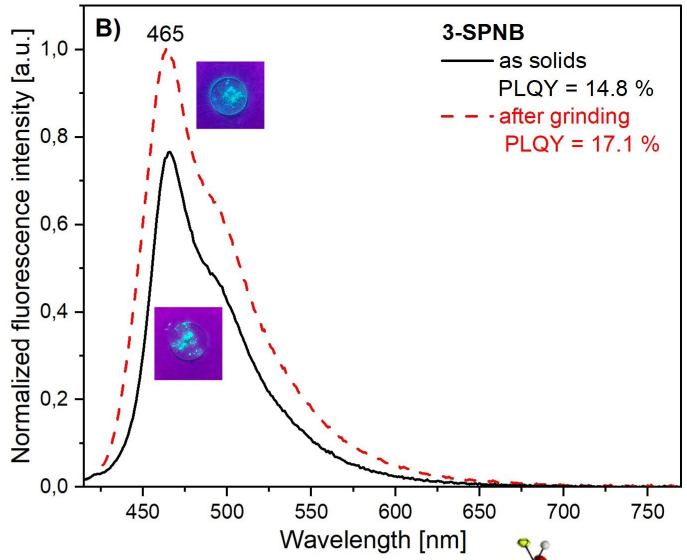
- ✓ *The emission of the long-lived component appears at 479 (**4-SPNB**) and 466 nm (**3-SPNB**), referred to the locally excited-state.*
- ✓ *The short-lived component appears at 487 and 479 nm, assigned to the PICT due to the rotation.*

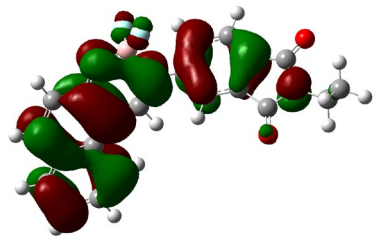


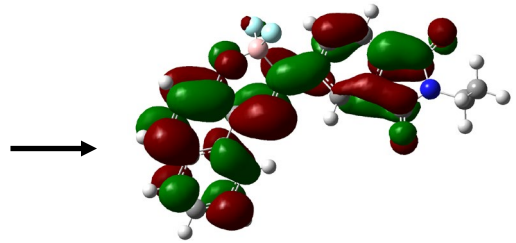
Time-resolved emissions spectra (TRES) in MeCN for 4-SPNB (A) and 3-SPNB (B).

- ✓ *The low energy emission bands depopulating first.*
- ✓ *The high energy bands are responsible for the later emission.*


A)
4-SPNB
as solids
PLQY = 13.27 %
after grinding
PLQY = 16.7 %
after fuming by DCM
510
468
Mechanochromism
Normalized fluorescence intensity [a.u.]
Wavelength [nm]

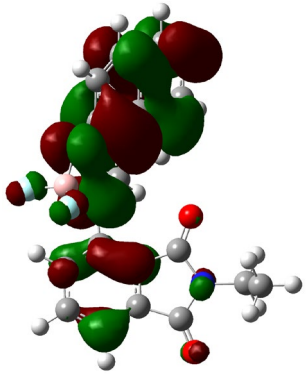

B)
3-SPNB
as solids
PLQY = 14.8 %
after grinding
PLQY = 17.1 %
465
Normalized fluorescence intensity [a.u.]
Wavelength [nm]

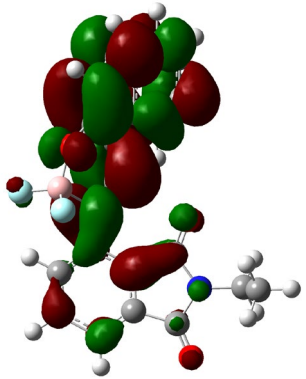


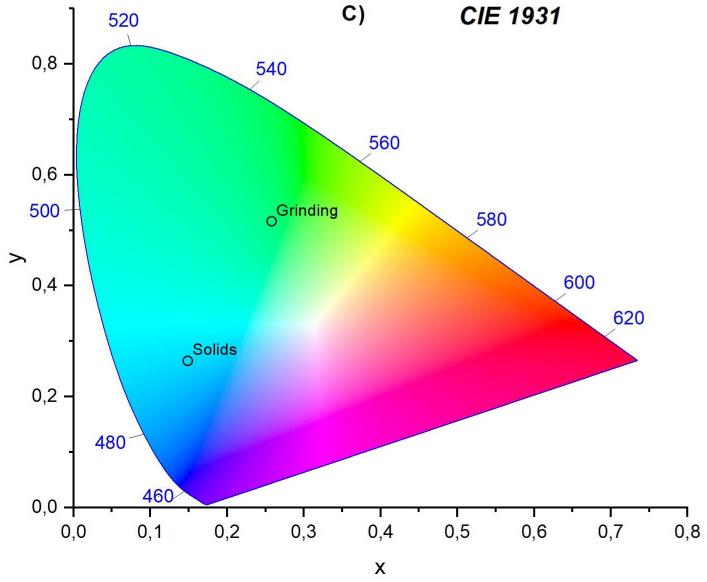


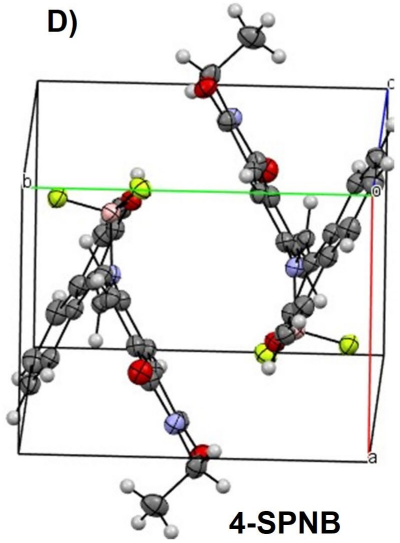
HOMO

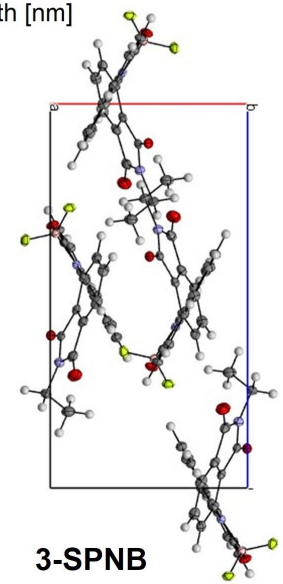
LUMO



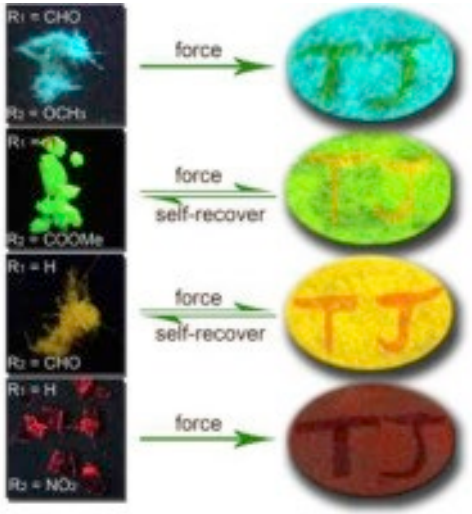



C)
CIE 1931
Grinding
Solids
x
y

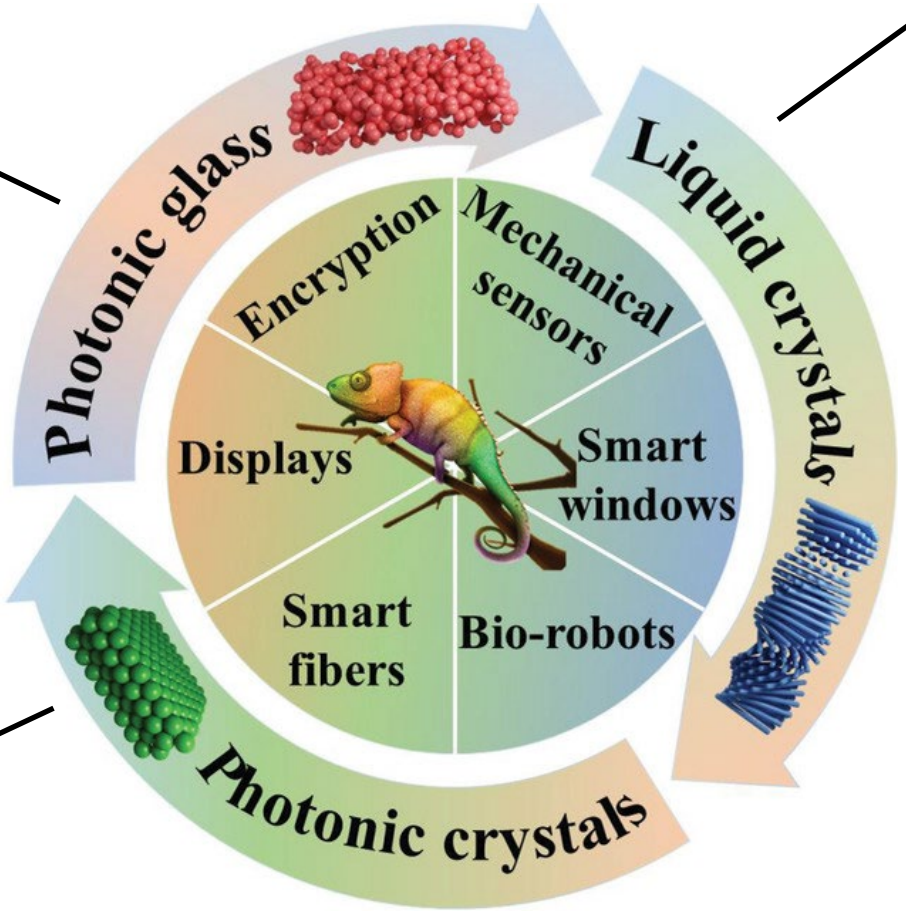

D)
4-SPNB

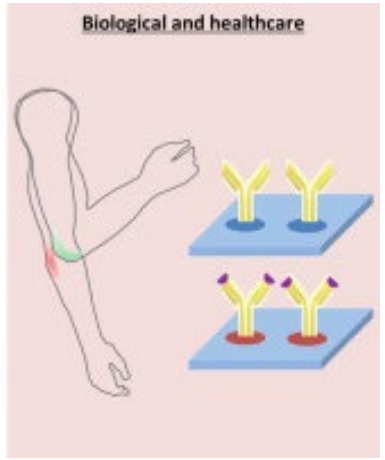

3-SPNB

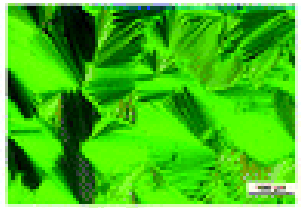
Mechanochromism – Applications



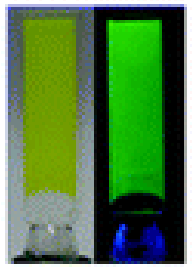
HiTech



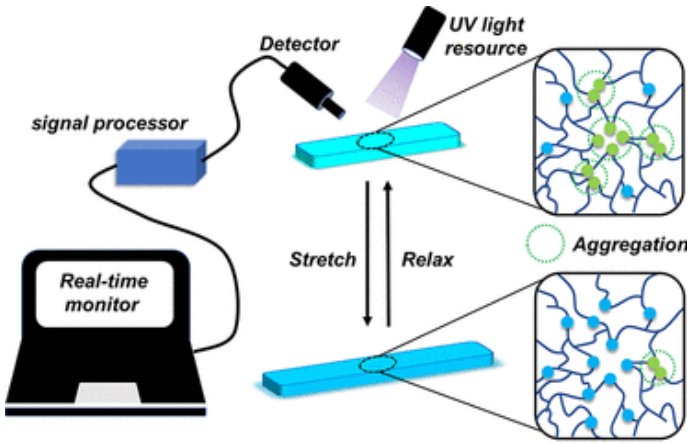




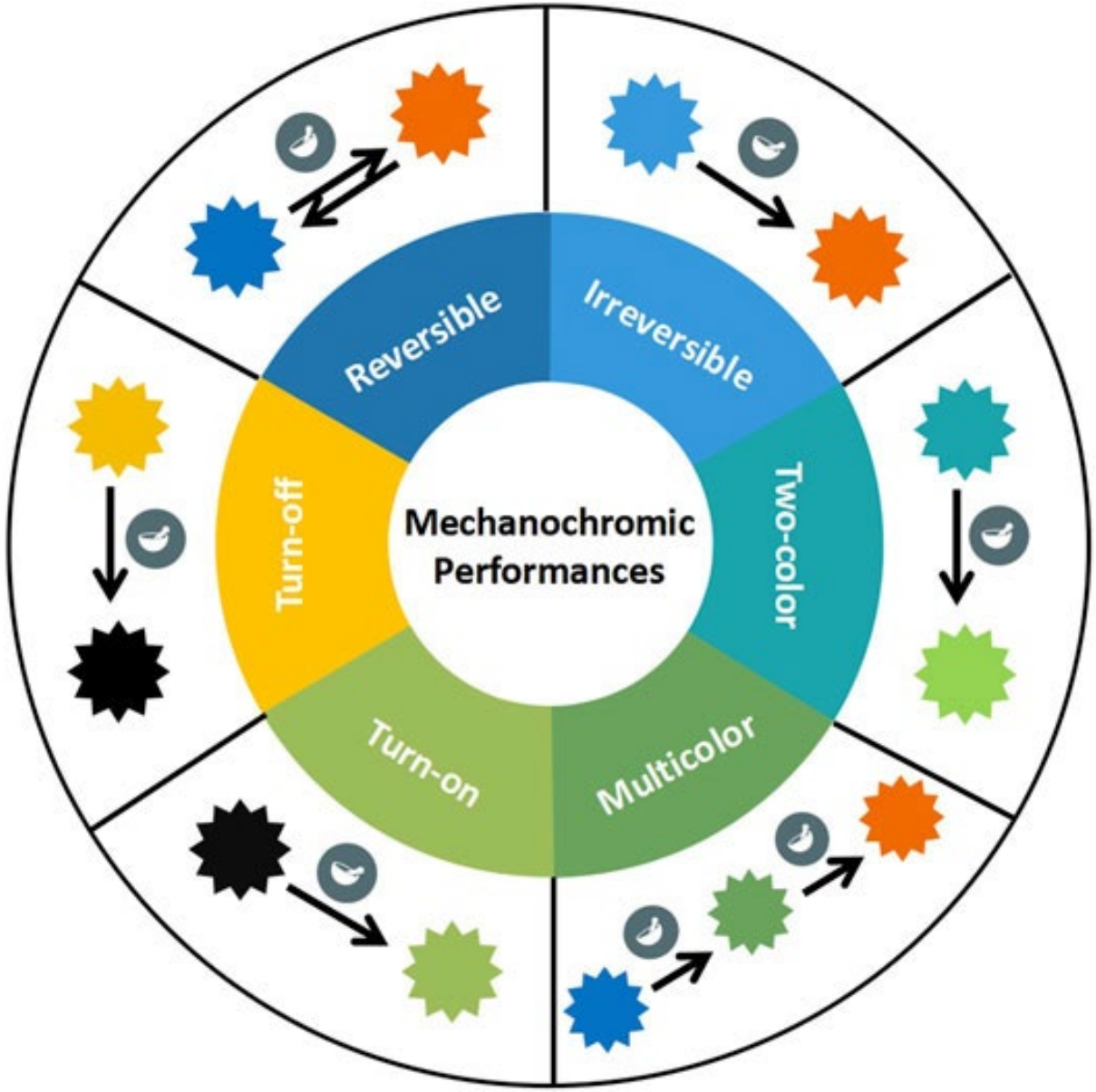
Liquid crystals



Gels



Mechanochromism - Applications



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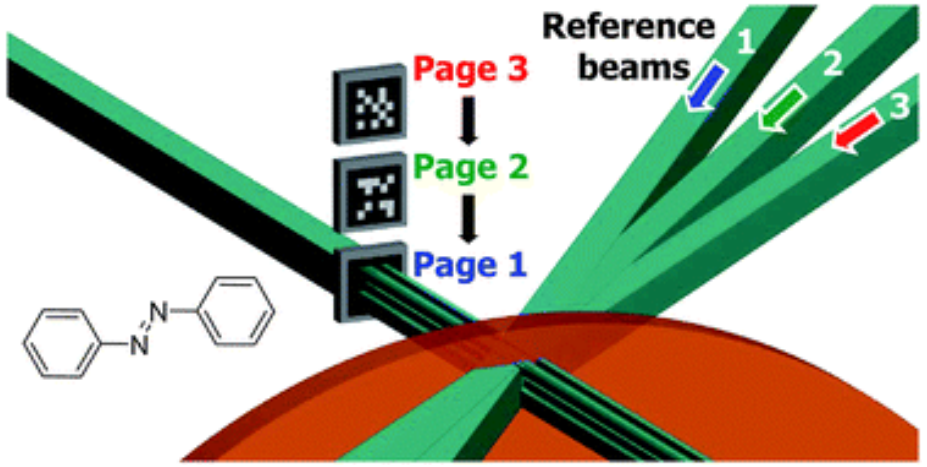
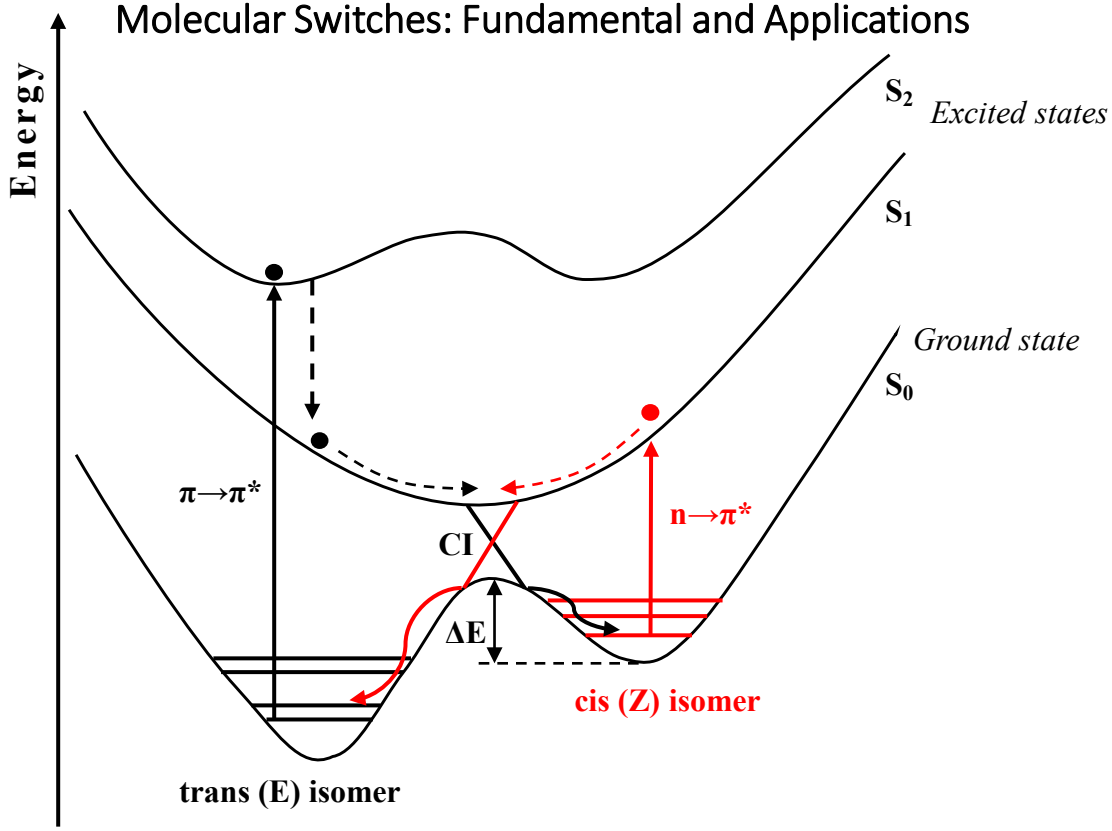
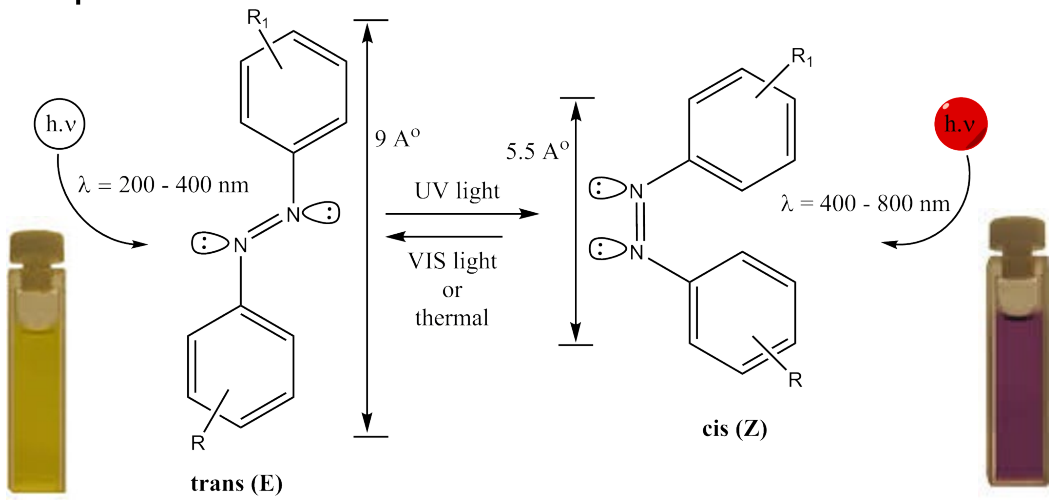
Photoanisotropic materials for polarization holography and photonics applications

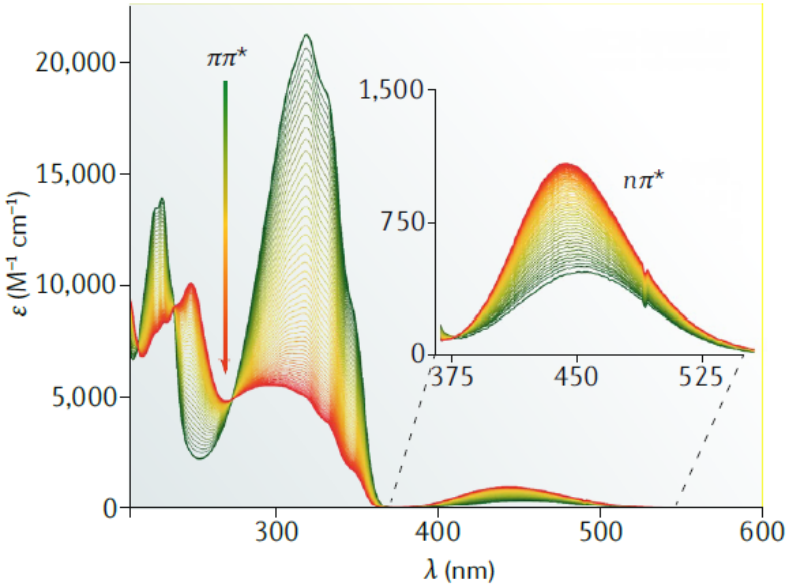


Molecular Switches: Fundamental and Applications

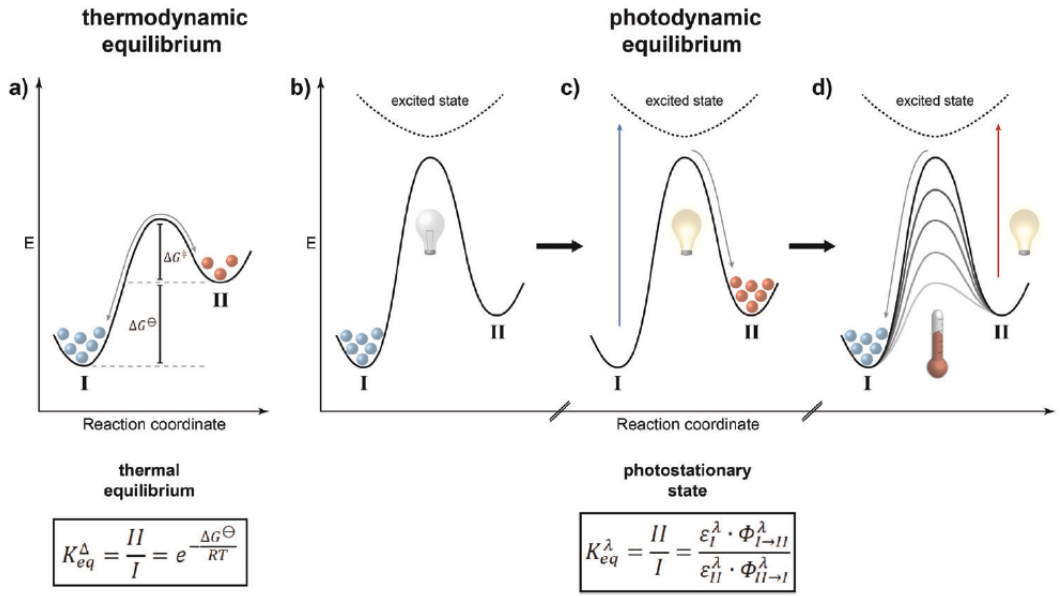




A. Georgiev et.al., Spectrochim. Acta. Part A. Mol. Biomol Spectrosc.175, 76-91 (2017)

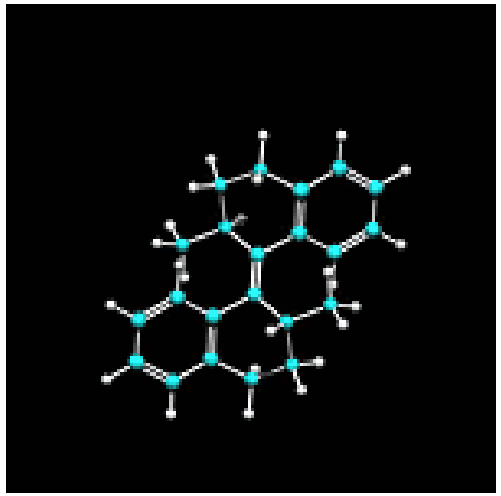


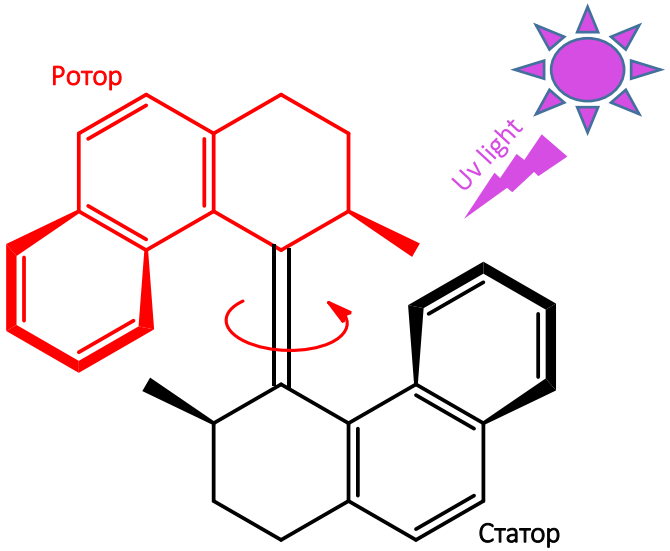
S. Crespi et.al., Nature Reviews Chemistry (2019)

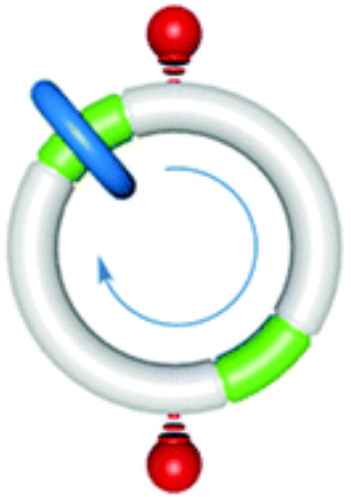


M. Kathan et.al., Nature Chemistry 10, 1031-1036 (2018)

Molecular switches: Who has the greatest fundamental contributions?



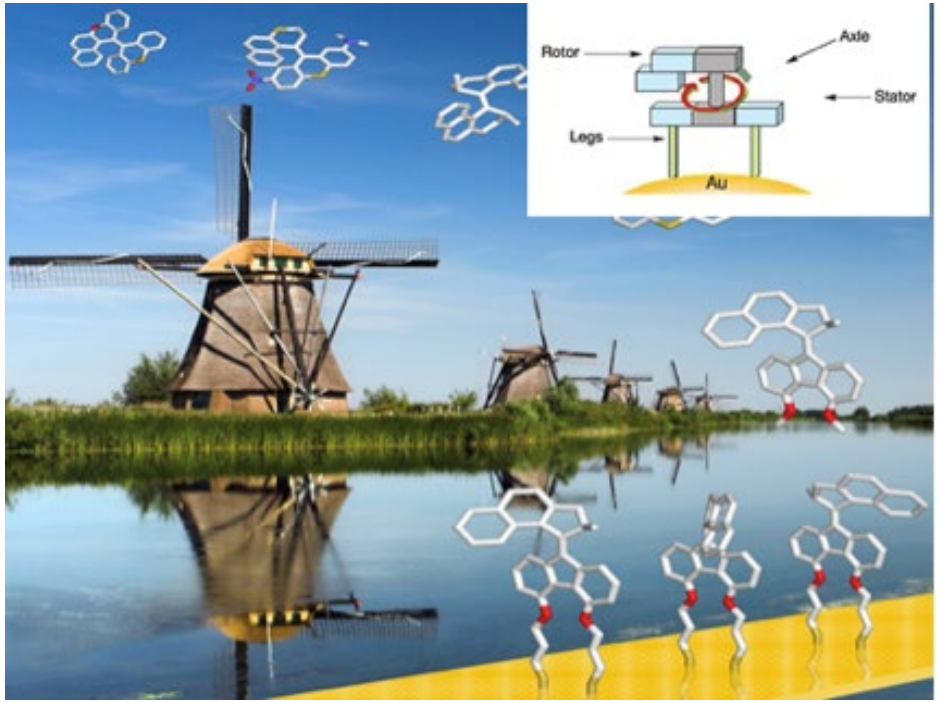


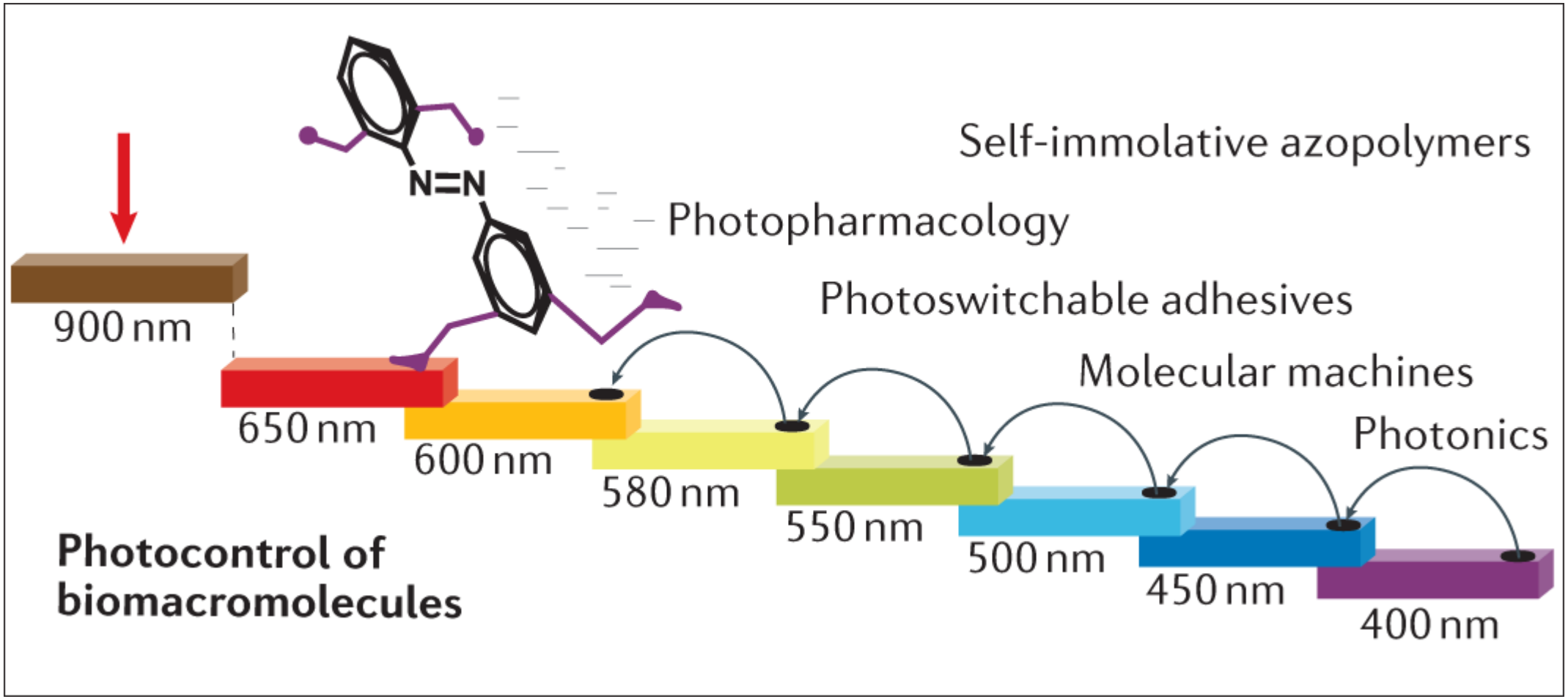


Ben Feringa
Nobel Prize in Chemistry 2016 y for the design and synthesis of molecular machines.

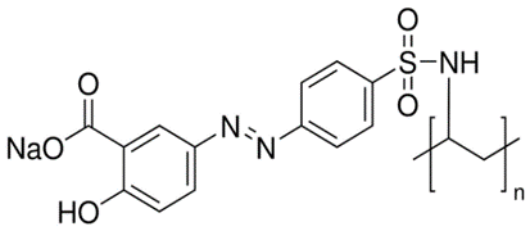
"Why does mankind need to fly? Why do we need molecular motors or machines? Nobody would have predicted that in the future one would build passenger planes each carrying several hundred people at close to the speed of sound between continents".

B. Feringa, nobel lecture 2017



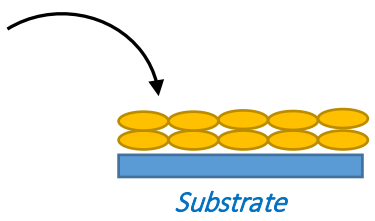

N=N
Self-immolative azopolymers
Photopharmacology
Photoswitchable adhesives
Molecular machines
Photonics
900 nm
650 nm
600 nm
580 nm
550 nm
500 nm
450 nm
400 nm
Photocontrol of biomacromolecules

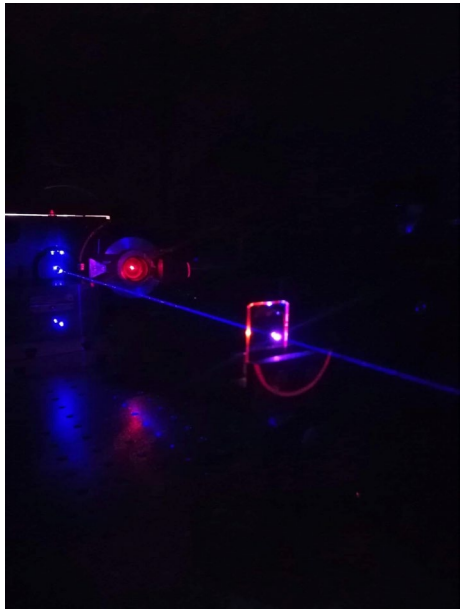
PAZO polymer: Optical anisotropy induced at five different wavelengths

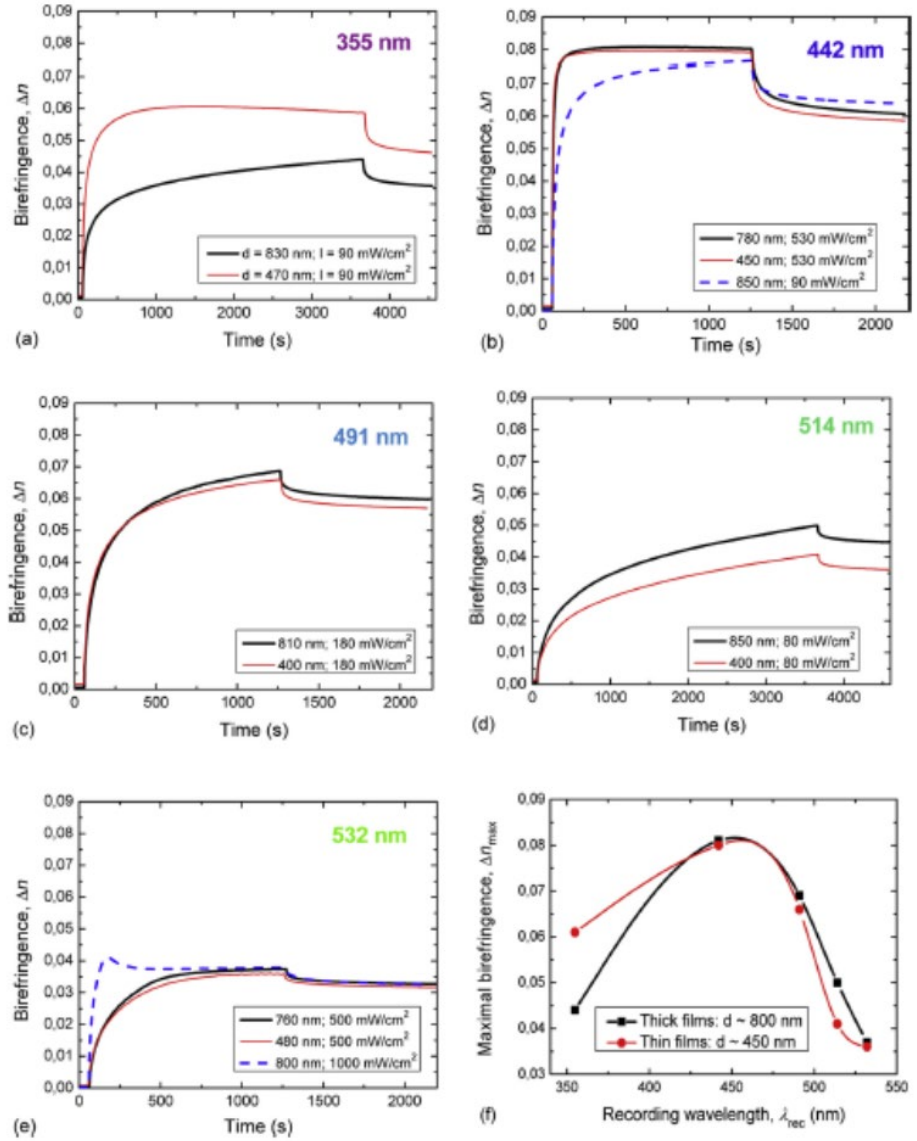


Poly[1-[4-(3-carboxy-4 hydroxyphenylazo) benzenesulfonamido]-1,2- ethanediyl, sodium salt]

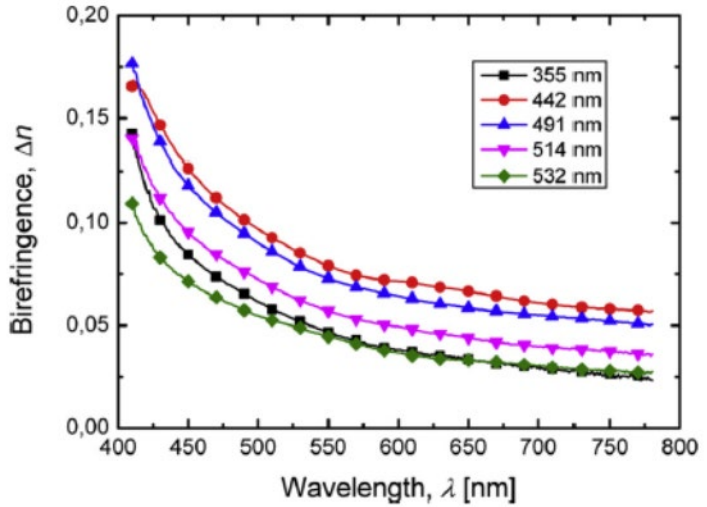
Film deposition of PAZO







Kinetics of birefringence recording and relaxation for the five pump lasers with wavelengths: (a) 355nm, (b) 442nm, (c) 491nm, (d) 514nm, and (e) 532nm; (f) Dependence of the maximal birefringence on the recording wavelength.



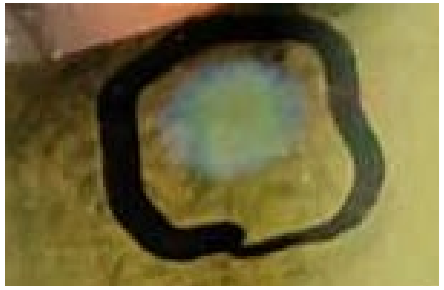
Spectral dependence of the birefringence induced at five different pump laser wavelengths.

L. Nedelchev et.al., J. Photochem. & Photobio. A: Chemistry 376 1-6 (2019)

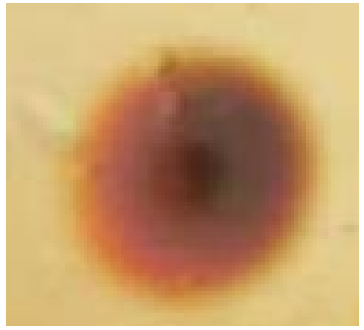
Diffraction gratings replication

Diffraction grating inscribed in the azopolymer PAZO with grating period 1 µm

Original grating, recorded holographically in azopolymer



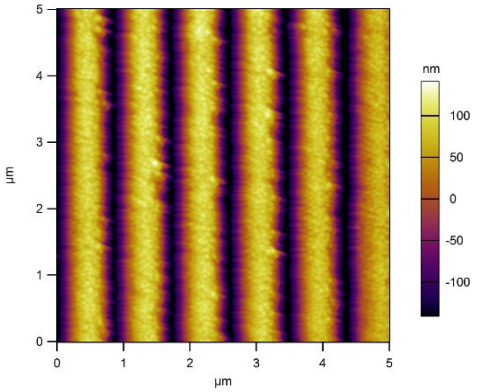
Replica of the grating obtained using silver and aluminum layers

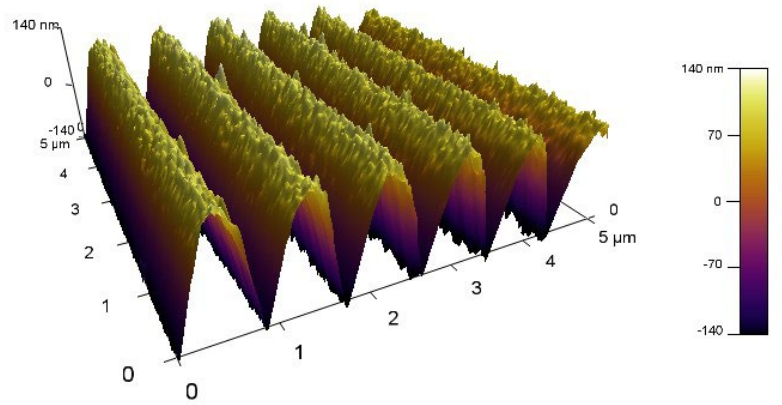


Atomic force microscopy (AFM)

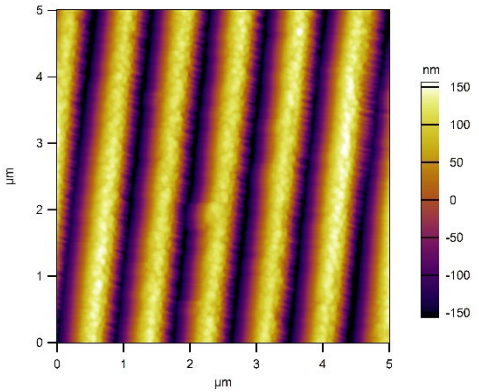
Diffraction grating inscribed in the azopolymer PAZO with grating period 1 µm

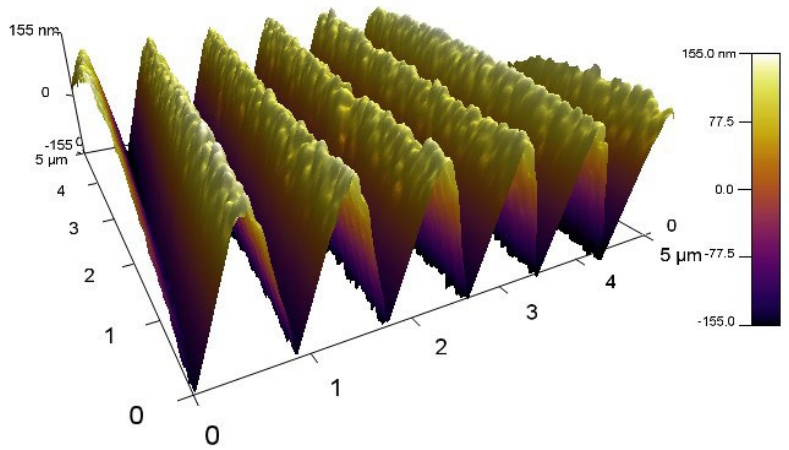
Original grating, recorded holographically in azopolymer





Replica of the grating obtained using silver and aluminum layers





Applications:

- Gas sensors
- Real-time visualization of biological tissue and photopharmacology
- Blood glucose sensor
- Optical transmitters

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