

Supporting Information

Light-Switchable One-Dimensional Photonic Crystals based on MOFs with Photomodulatable Refractive Index

Zejun Zhang,^{a,#} Kai Müller,^{a,#} Shahriar Heidrich,^{b,#} Meike Koenig,^a Tawheed Hashem,^a Tobias Schlöder,^b David Bléger,^c Wolfgang Wenzel,^b Lars Heinke^{a,}*

^a Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany.

^b Institute of Nanotechnology (INT), KIT, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany.

^c Department of Chemistry & IRIS Adlershof Humboldt-Universität zu Berlin, 12489 Berlin, Germany. Present affiliation: Evonik Creavis GmbH, Paul-Baumann-Straße 1, 45772 Marl, Germany.

[#] These authors contributed equally.

IRRAS Data

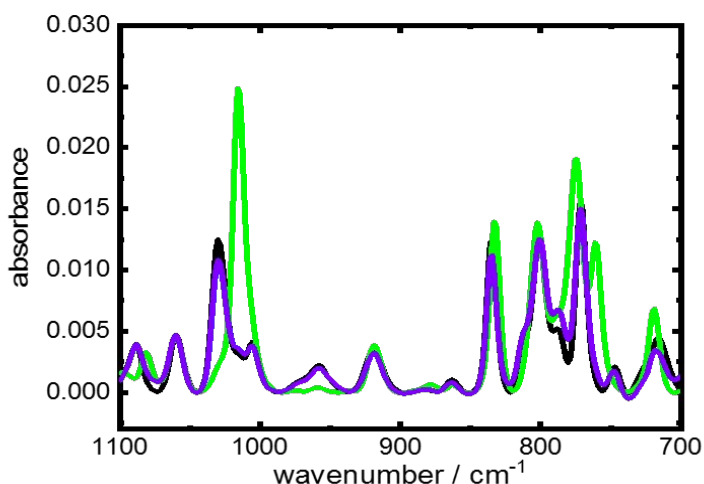


Figure SI1: Infrared spectra of the thermally relaxed sample (black, 100% *trans*), upon 530 nm (green, *cis*) and upon 400 nm (violet, *trans*) irradiation. The black and violet spectra are almost identical.

Experimental Spectroscopic Ellipsometry Data

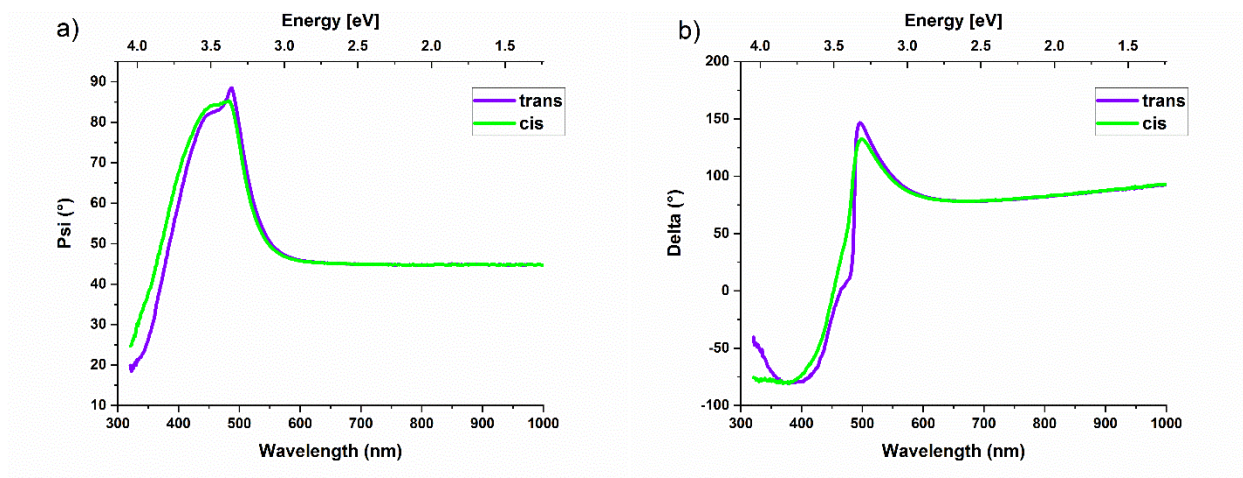


Figure S12: Raw experimental spectra of the ellipsometric angles Psi (a) and Delta (b) of the photoswitchable SURMOF after irradiation with green (*cis*) and violet (*trans*) light.

DFT Calculations

Table SII: Calculated excitation energies, oscillator strengths and main molecular orbital transition contributions for the two F₂AzoBDCH₂ isomers.

	Energy / eV	Energy / nm	Oscillator strength / a.u.	Main contribution
<i>trans</i>				
1	2.38439	519.983	0.00239	HOMO → LUMO (94%)
2	3.57726	346.589	0.01471	HOMO → LUMO+1 (92%)
3	3.78861	327.255	0.58989	HOMO-1 → LUMO (87%)
<i>cis</i>				
1	2.65216	467.484	0.03585	HOMO → LUMO (77%)
2	3.34871	370.244	0.01449	HOMO → LUMO+1 (77%)
3	3.96250	312.894	0.00488	HOMO-1 → LUMO (95%)

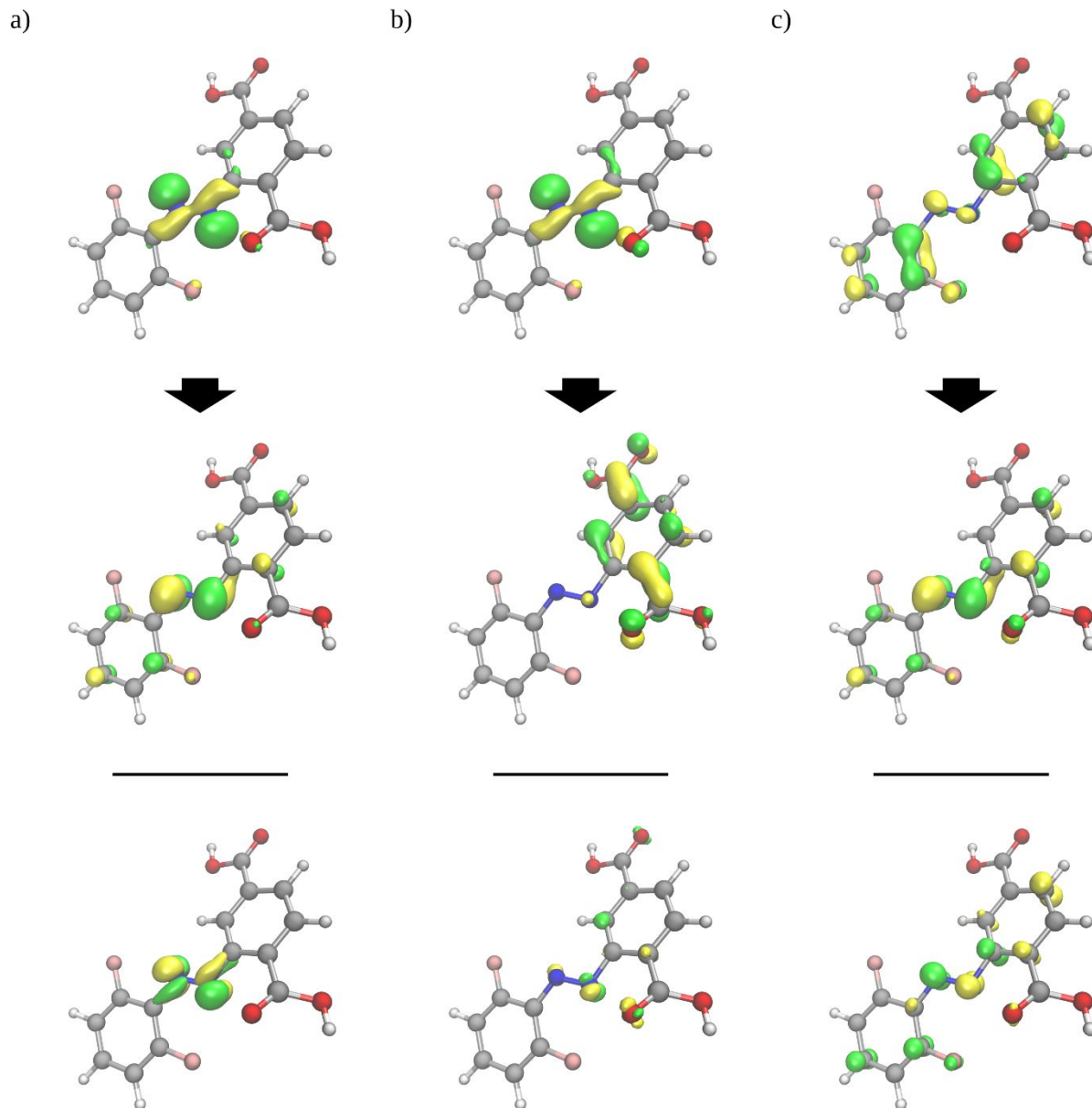


Figure SI3: Calculated transition orbitals and transition densities for the three lowest-lying excitations of *trans*-F₂AzoBDCH₂. (a), (b) and (c) correspond to excitations 1, 2 and 3, respectively, in Table SI1. Holes resulting from the excitations are shown in the upper row, the corresponding electrons in the middle row. Yellow and green indicate negative and positive phase, respectively. The bottom row shows the associated transition densities. Here, yellow and green indicate negative and positive phase, respectively.

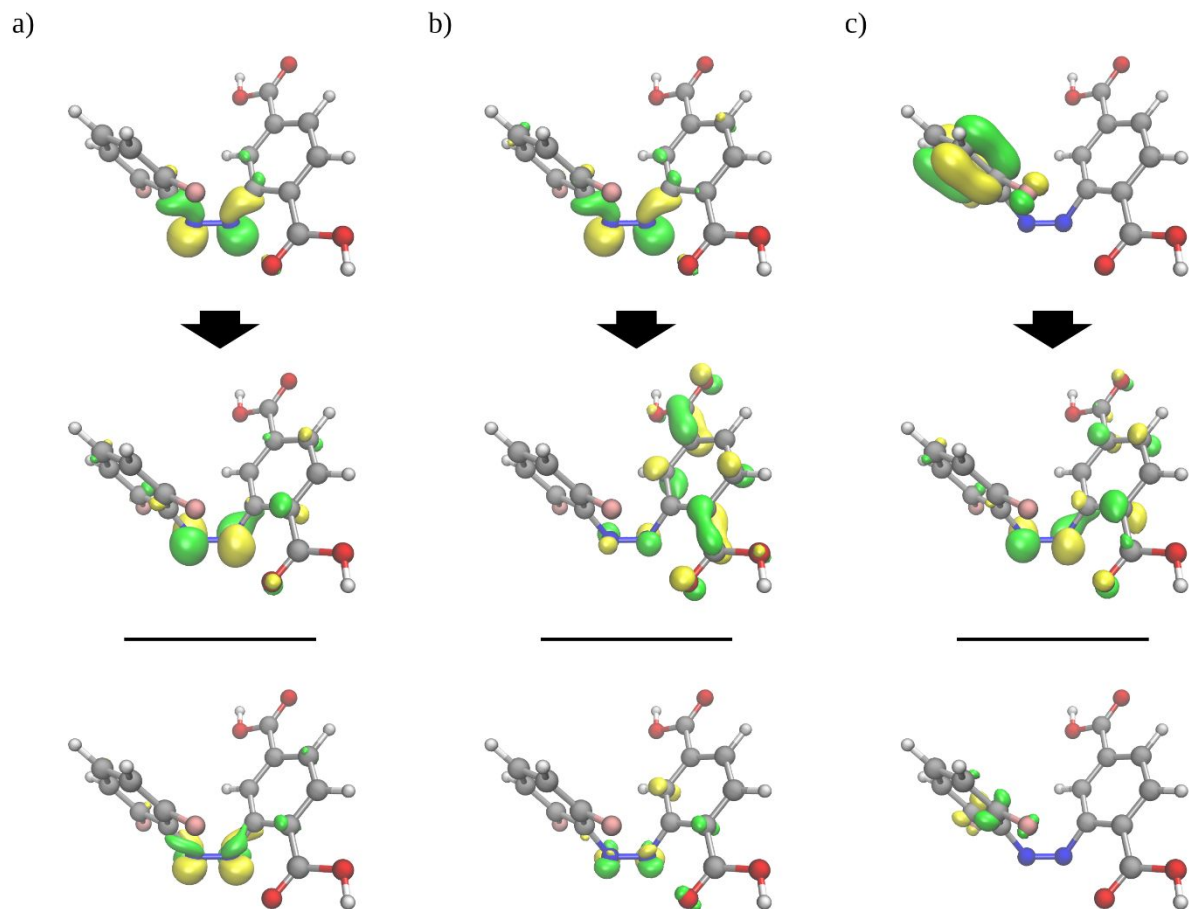


Figure SI4: Calculated transition orbitals and transition densities for the three lowest-lying excitations of *cis*-F₂AzoBDCH₂. (a), (b) and (c) correspond to excitations 1, 2 and 3, respectively, in Table SI1. Holes resulting from the excitations are shown in the upper row, the corresponding electrons in the middle row. Yellow and green indicate negative and positive phase, respectively. The bottom row shows the associated transition densities. Here, yellow and green indicate negative and positive phase, respectively.