

SUPPORTING INFORMATION

Photoinduced structural modifications in multicomponent architectures containing azobenzene moieties as photoswitchable cores

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I - Crystallographic data

Table S1. X-ray diffraction data for molecule **2**.

Formula	C ₅₂ H ₆₈ N ₄
<i>M_r</i>	749.1
Crystal system	triclinic
Space group	<i>P</i> $\bar{1}$
<i>a</i> / Å	11.2511(7)
<i>b</i> / Å	12.407(1)
<i>c</i> / Å	17.793(1)
α / °	96.813(4)
β / °	91.644(5)
γ / °	116.369(6)
<i>V</i> / Å ³	2200.3(3)
Z	2
<i>D_c</i> / g cm ⁻³	1.131
μ / mm ⁻¹	0.492
<i>F</i> (000)	816
<i>R</i> (int)	0.080
θ range / °	5.00 - 54.16
No. of data collected	7070
No. of unique data	4871
No. of observed data [<i>I</i> > 2 σ (<i>I</i>)]	3556
Goodness of fit	0.971
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2 σ (<i>I</i>)]	0.0469, 0.1045
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.0668, 0.1105

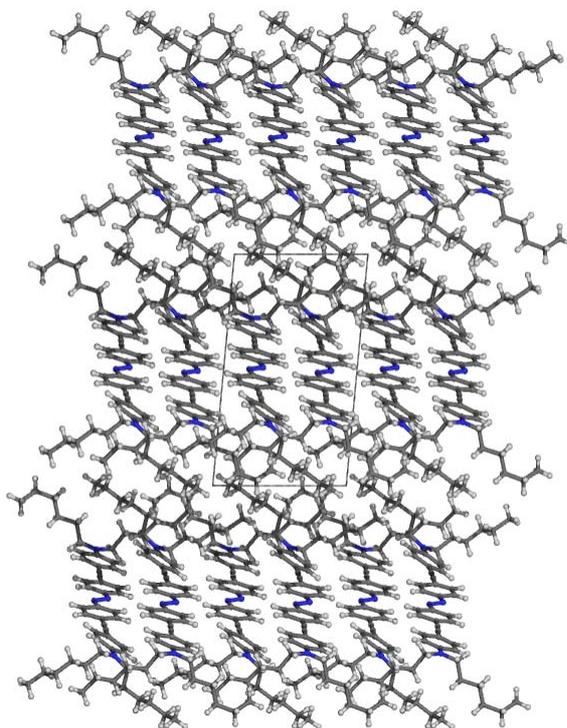


Fig. S1 Crystal packing of molecule **2** along the *y* crystallographic direction.

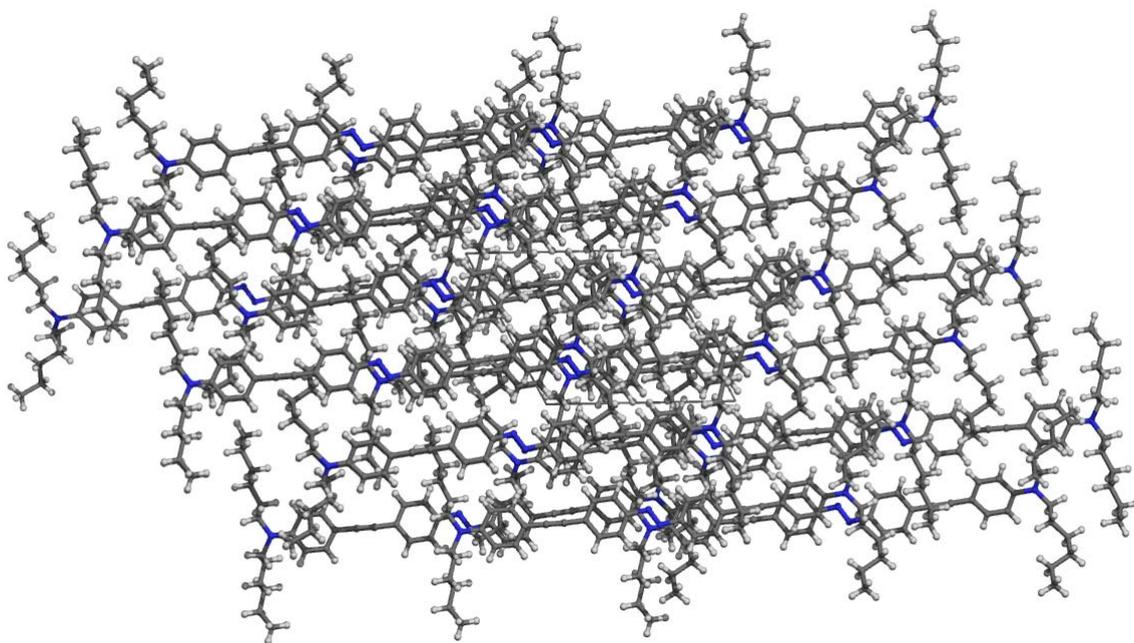


Fig. S2 Crystal packing of molecule **2** along the *z* crystallographic direction.

II - Photochemistry

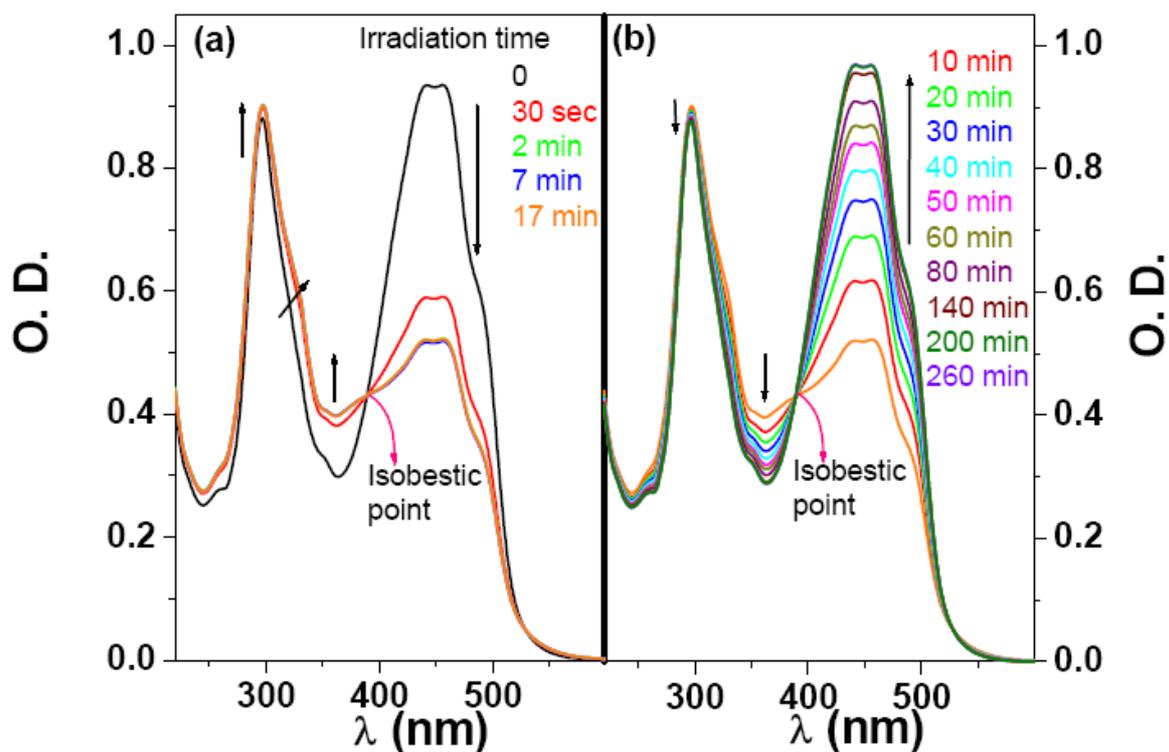


Fig. S3 (a) Time evolution of the absorption spectra of a $2.2 \times 10^{-4} \text{ M}^{-1}$ solution of *trans*-2 in CHX under 450 nm light irradiation, until the photostationary state is reached. (b) Thermal back reaction in the dark.

III - Additional microscopic information

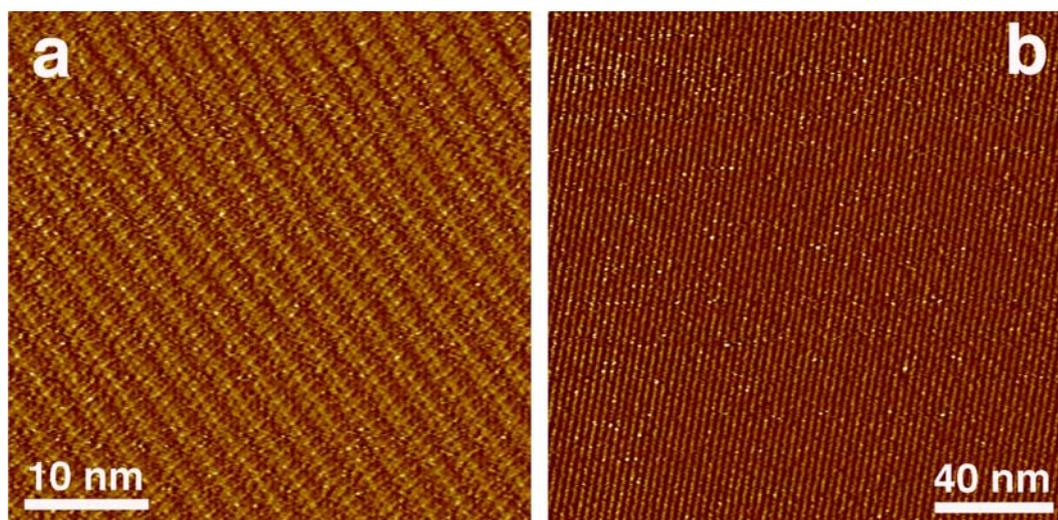


Fig. S4 Constant Height STM images of the SAM formed by *trans*-**2** at the HOPG-Phenylloctane interface. Tunneling conditions: average tunneling current (I_t)=10 pA, bias voltage (V_t)=500 mV.

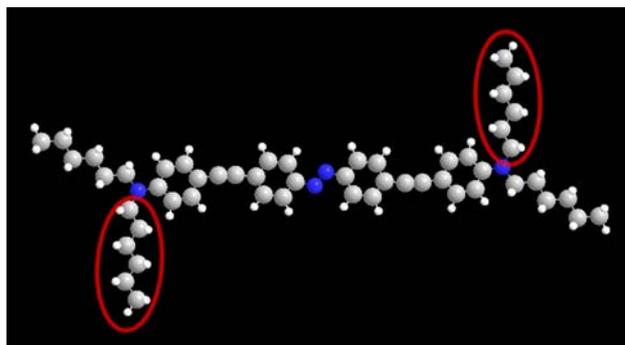


Fig. S5 CPK model of **2** molecule highlighting the alkyl chain branches that are most likely not physisorbed on HOPG.

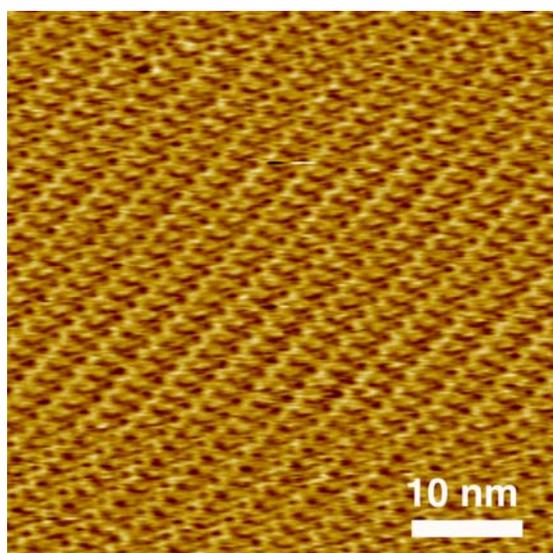


Fig. S6 STM image of the **2** SAM after 3 hours of irradiation *ex-situ*. Tunneling conditions: (I_t) =10 pA, (V_t)=500 mV.

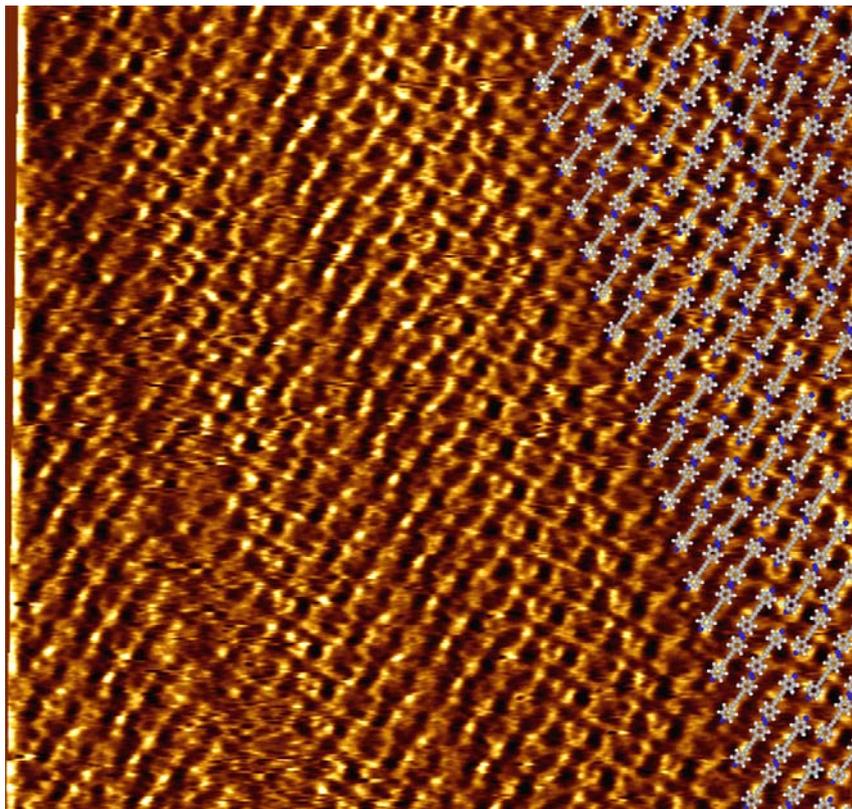


Fig. S7 STM current image of the SAM formed by *trans*-**3** in 1-phenyloctane at the HOPG-solution interface (N'-Alkyl chains are not shown for clarity). Image size: 23×24 nm². Tunneling conditions: average tunneling current (I_t) = 10 pA, bias voltage (V_t) = 300 mV. The CPK molecular models and the unit cell are superimposed.