Electronic Supplementary Information (ESI)

Observance of a large conformational change associated with the rotation of the naphthyl groups during the photodimerization of criss-cross aligned C=C bonds within a 2D coordination polymer

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Experimental

1. Preparation of 4-spy, (E)-4-(2-(naphthalen-2-yl)vinyl)pyridine 4-(2-npy) and (E)-4-(2-(naphthalen-1-yl)vinyl)pyridine (4-npy). Corresponding bromomethyl derivatives were treated with triphenylphosphine in toluene. The resulting product mixed with pyridylaldehyde in sodium hydrate solution and stirred for 20h. The crude product was obtained by evaporation of the solvents in vacuo. The mixture was loaded on a column filled with silica gel and eluted with ethyl acetate / mineral ether (2:1). $^1$H NMR (400MHz, DMSO, TMS): 4-spy, $\delta$ 8.56 (d, 2H, py-H), 7.6 (d, 2H, py-H), 8.57 (d, 2H, Ph-H) 7.56 (d, 1H, C=C), 7.3-7.4 (m, 5h, Ph-H), 7.28 (d, 1H, C=C). 4-(2-npy), $\delta$ 8.6 (d, 2H, py-H), 8.1 (s, 1H, naphthalene-H), 7.9 (m, 4H, naphthalene-H), 7.7(1H, C=C), 7.6(2H, py-H), 7.5(2H, naphthalene-H), 7.4(1H, C=C). 4-npy, $\delta$ 8.6 (d, 2H, py-H), 8.46 (d, 1H, naphthalene-H), 8.39 (d, 1H, C=C), 7.94 (m, 5h, naphthalene-H), 7.75 (dd, 2H, py-H), 7.59 (m, 5h, naphthalene-H), 7.32 (d, 1H, C=C) (Figures S1).

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Gas phase structure optimizations were carried out using DFT as implemented in the Gaussian 09 package with the B3LYP functional using 6-31G* basis sets.$^1$

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