Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information for

The investigation of hydrogen bond saturation effect during the dipole induced azobenzene supramolecular self-assembly

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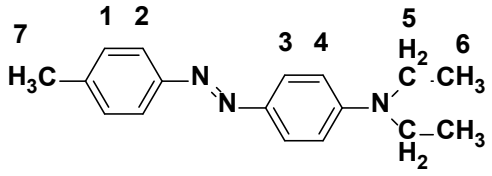
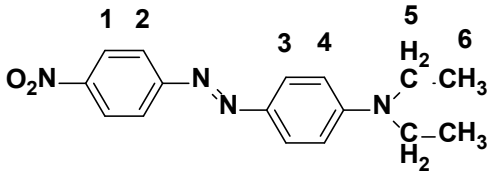


N1

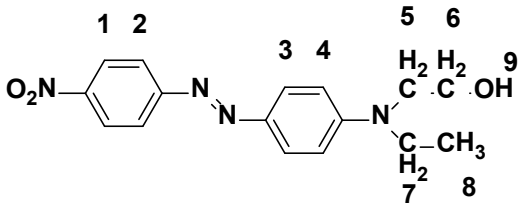
N1: IR (KBr), υ /cm^{-1}: 2970 (-CH_3), 2890 (-CH_2), 1596, 1512 (Ar), 1450 (-N=N-). δ_H(400 MHz, $CDCl_3$; Me_4Si) 1.251 - 1.215 (2H, t, *J* = 7.6 Hz, 6-H), 2.410 (3H, s, 7-H), 3.480 - 3.428 (4H, q, 5-H), 6.735 - 6.715 (2H, d, *J* = 8.0 Hz, 4-H), 7.277 - 7.257 (4H, d, *J* = 8.0 Hz, 1-H), 7.754 - 7.734 (4H, d, *J* = 8.0 Hz, 3-H), 7.857 - 8.836 (4H, d, *J* = 7.6 Hz, 2-H). δ_C(400 MHz, $CDCl_3$; Me_4Si) 12.6, 21.4 (CH_3), 44.6 (CH_2), 110.9, 122.0, 125.1, 129.5, 139.4.2, 143.0.4, 149.8, 151.3 (Ph). Found: C, 76.26; H, 6.31; N, 19.76. Calc. for $C_{17}N_3H_{21}$: C, 76.37; H, 6.20; N, 19.89%.



N2

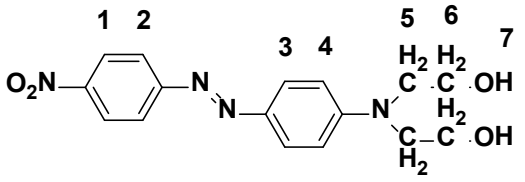
N2: IR (KBr), υ /cm^{-1}: 2970 (-CH_3), 2925 (-CH_2), 1601, 1520 (Ar), 1450 (-N=N-), 1506, 1343(-NO_2). δ_H(400 MHz, $CDCl_3$; Me_4Si) 1.286 - 1.250 (6H, t, J=7.4

Hz, 6-H), 3.528 - 3.474 (4H, q, 5-H), 6.790 (2H, d, 4-H), 7.948 - 7.926 (4H, d, J=8.8 Hz, 1, 2-H), 8.337 - 8.314 (2H, d, J=9.2 Hz, 3-H). δ_C(400 MHz, $CDCl_3$; Me_4Si) 12.6 (CH_3), 44.9 (CH_2), 110.7, 122.5, 124.7, 126.5, 143.2, 147.1, 151.3, 156.9 (Ph). Found: C, 64.20; H, 6.13; N, 18.90. Calc. for $C_{16}N_4H_{18}O_2$: C, 64.41; H, 6.08; N, 18.78%.



N3

N3: IR (KBr), υ /cm^{-1}: 3496 (OH), 2948 (-CH_3), 2915 (-CH_2), 1601,1513 (Ar), 1421 (-N=N-), 1513,1331 (-NO_2). δ_H(400 MHz, $CDCl_3$; Me_4Si) 1.287 - 1.252 (3H, t, J=6.9 Hz, 8-H), 1.750 (2H, s, 9-H), 3.613 - 3.559 (2H, q, 7-H), 3.652 - 3.623(2H, d, J = 6.0 Hz, 6-H), 3.922 - 3.893 (2H, d, J = 6.0 Hz, 5-H), 6.864 - 6.843(2H, d, J = 8.4 Hz, 4-H), 7.950 - 7.932 (2H, d, J = 7.2 Hz, 2-H), 7.928 - 7.910(2H, d, J = 7.2 Hz, 1-H), 8.339 - 8.316 (2H, d, J = 9.2 Hz, 3-H). δ_C(400 MHz, $CDCl_3$; Me_4Si) 12.1 (CH_3), 45.9, 52.3, 60.3 (CH_2), 111.5, 122.6, 124.7, 126.2, 143.7, 147.3, 151.6, 156.7 (Ph). Found: C, 61.23; H, 5.89; N, 17.69. Calc. for $C_{16}N_4H_{18}O_3$: C, 61.13; H, 5.77; N, 17.82%.



N4

N4: IR (KBr), υ /cm^{-1}: 3277 (OH), 2961 (-CH_3), 2925 (-CH_2), 1598,1513 (Ar), 1424 (-N=N-), 1513,1334 (-NO_2). δ_H(400 MHz, $CDCl_3$; Me_4Si) 1.555 (2H, s, 7-H), 3.692 - 3.665 (4H, s, J=5.6, 6-H), 3.925 - 3.898 (4H, s, J=5.6, 5-H), 6.869 - 6.848(2H, d, J = 8.8 Hz, 4-H), 7.960 - 7.938(4H, d, J = 8.8 Hz, 1, 2-H), 8.343 - 8.321(2H, d, J =

8.8 Hz, 3-H).δ_C(400 MHz, $CDCl_3$; Me_4Si) 60.3, 54.6 (CH_2), 111.8, 122.6, 124.7, 126.2, 143.9, 147.4, 152.8, 156.6 (Ph). Found: C, 58.30; H, 5.31. Calc. for $C_{16}N_4H_{18}O_4$: C, 58.17; H, 5.49; N, 16.96; N 17.13%.

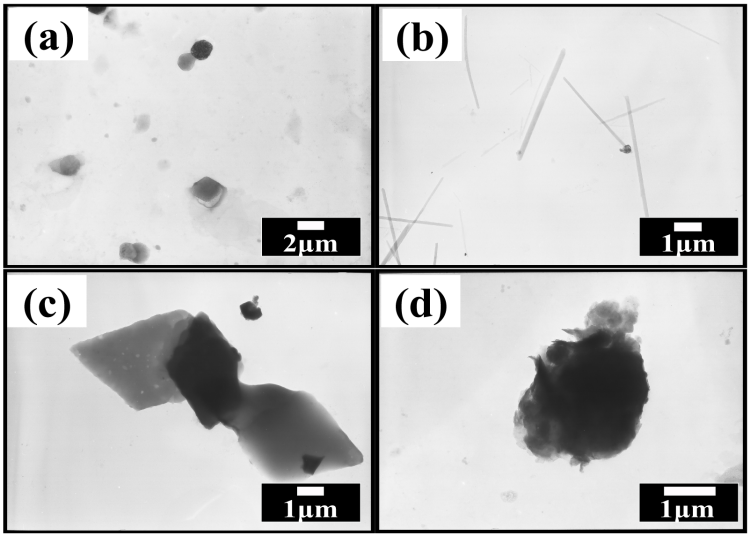
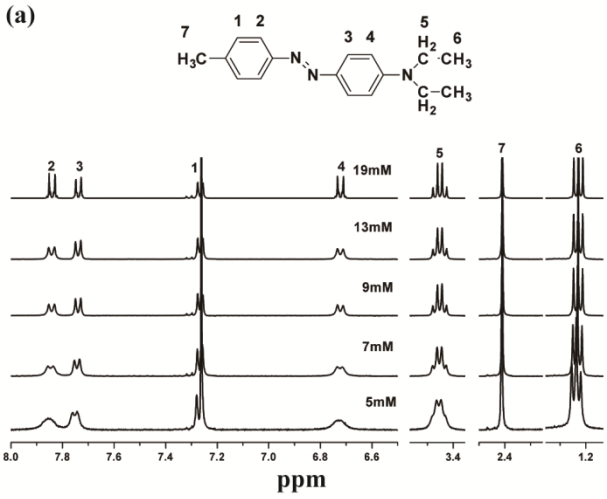


Fig S1. TEM image of the self-assembly nanostructure at RT and pH 7, (a) N1, (b) N2, (c) N3 and (d) N4.



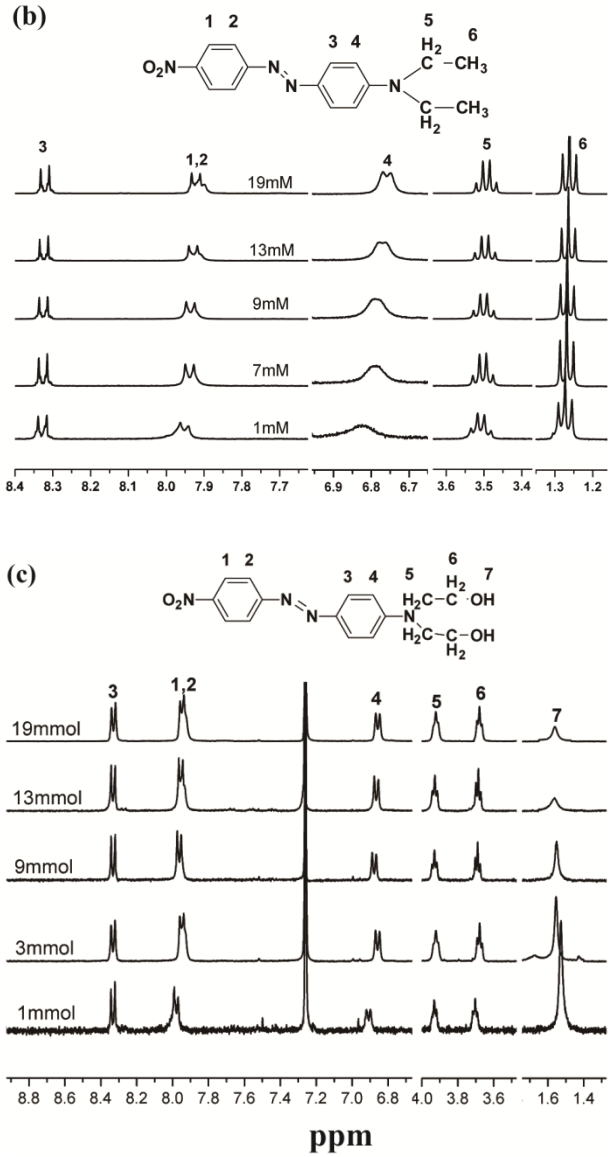


Fig S2. ^{1}H NMR spectra of (a) N1, (b) N2, (c) N4 at different concentrations in $CDCl_3$

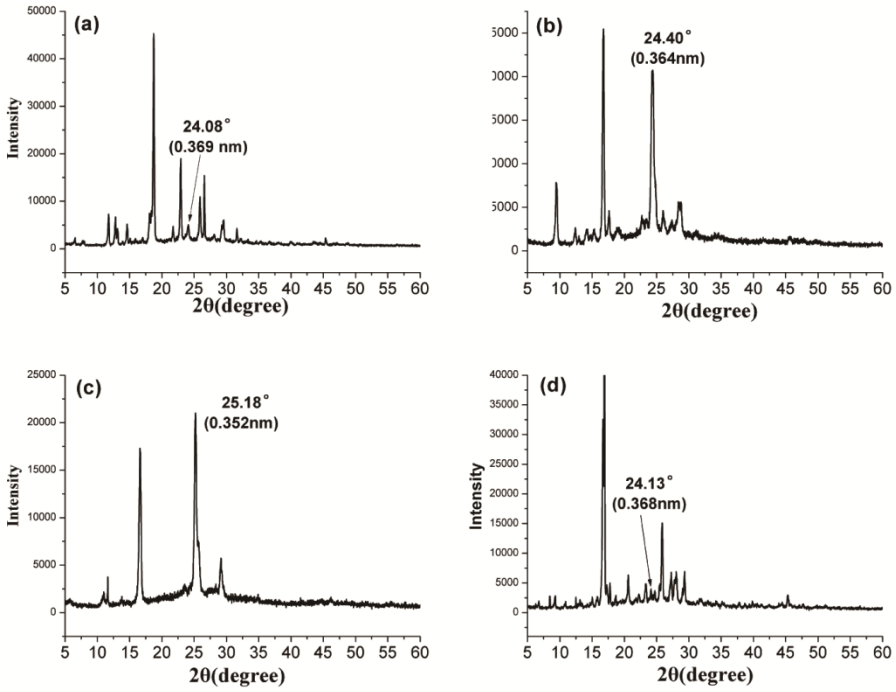
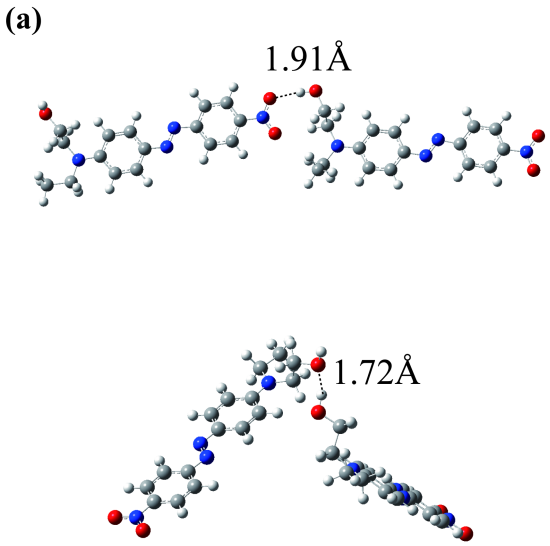


Fig S3. XRD spectra of (a) N1, (b) N2, (c) N3, (d) N4.



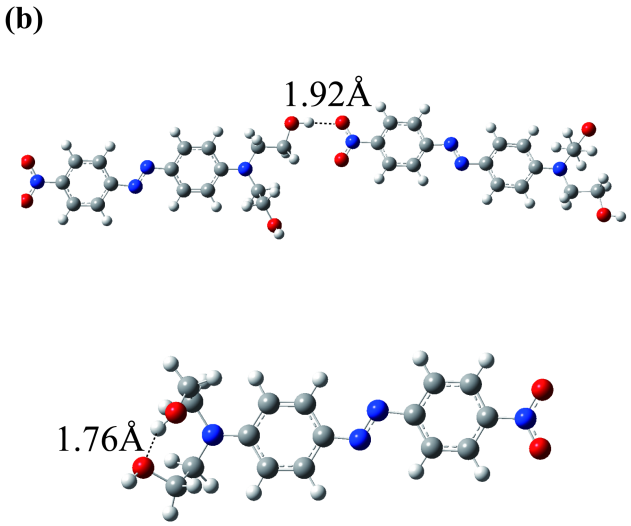


Fig S4. The hydrogen bonding distributions of (a) N3 and (b) N4 implemented on the Gaussian program.

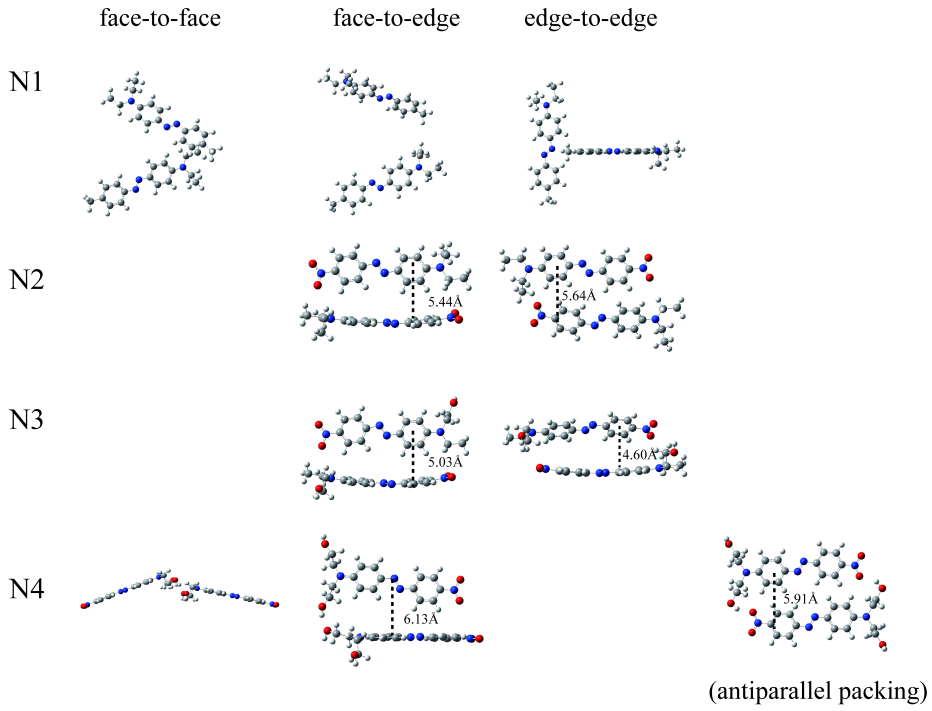


Fig S5. calculated molecular packing structures of azobenzene molecules.